Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.

Supporting information

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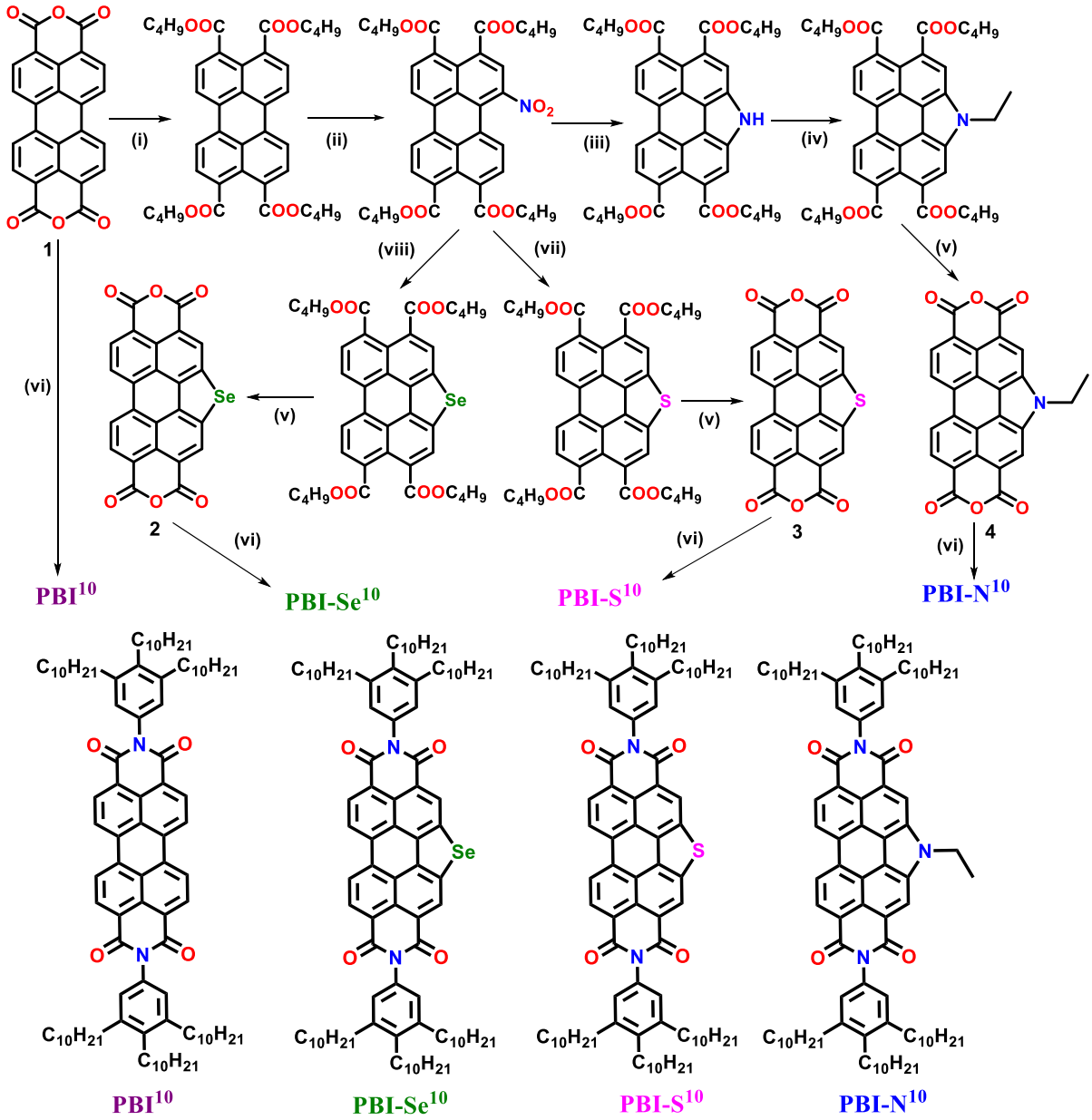
1. Materials and methods

Commercially available chemicals were used without any purification; solvents were dried following the standard procedures. Chromatography was performed using either silica gel (60-120 mesh) or neutral aluminium oxide. For thin layer chromatography, aluminium sheets pre-coated with silica gel were employed. IR spectra were recorded on a Perkin Elmer IR spectrometer at normal temperature by using KBr pellet. The spectral positions are given in wave number (cm^{-1}) unit. NMR spectra were recorded using Bruker 600 MHz NMR spectrometer. For ^{1}H NMR spectra, the chemical shifts are reported in ppm relative to TMS as an internal standard. Coupling constants are given in Hz. Mass spectra were determined from MALDI-TOF mass spectrometer using α-Cyano-4-hydroxycinnamic acid as a matrix or High Resolution Mass Spectrometer. The mesogenic compounds were investigated for their liquid crystalline behavior (birefringence and fluidity) by employing a polarizing optical microscope (Nikon Eclipse LV100POL) equipped with a programmable hot stage (Mettler Toledo FP90). Clean glass slides and coverslips were employed for the polarizing optical microscopic observations. The transition temperatures and associated enthalpy changes were determined by differential scanning calorimeter (Mettler Toledo DSC1) under nitrogen atmosphere. Peak temperatures obtained in DSC corresponding to transitions were in agreement with the polarizing optical microscopic observations. The transition temperatures obtained from calorimetric measurements of the first heating and cooling cycles at a rate of 5 °C/min are tabulated. X-ray diffraction measurements were carried out using image plate (IP) and a solid state detector. In this apparatus Cu K_{α} (λ =0. 15418 nm) radiation from a source (GeniX3D, Xenocs) operating at 50 kV and 0.6 mA in conjunction with a multilayer mirror was used to illuminate the sample, which was contained in a glass capillary tube (Capillary Tube Supplies Ltd). The temperature of the sample was varied using a Mettler hot stage/ programmer (FP82HT/FP90). The diffraction patterns were collected on a 2D IP detector of 345 mm diameter and 0.1 mm pixel size (Mar345, Mar Research). Thermogravimetric analysis (TGA) was performed using thermogravimetric analyzer (Mettler Toledo, model TG/SDTA 851 e) under a nitrogen flow at a heating rate of 10 °C/min. UV-Vis spectra were obtained by using Perkin-Elmer Lambda 750, UV/VIS/NIR spectrometer. Fluorescence emission spectra in solution state were recorded with Horiba Fluoromax-4 fluorescence spectrophotometer or Perkin Elmer LS 50B spectrometer. Cyclic Voltammetry studies were carried out using a Versa Stat 3 (Princeton Applied Research) Electrochemical workstation.

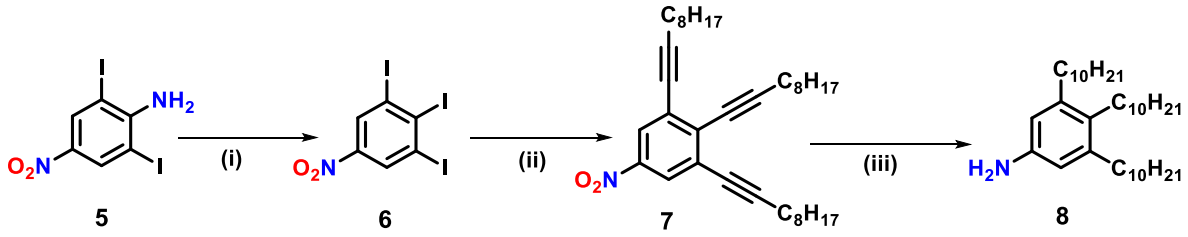
2. Experimental Section:

Scheme 1. Synthesis of bay-annulated PBIs



Scheme 1. Synthesis of bay-annulated perylene bisimides. Reagents and conditions: (i) KOH, H_2O, 70 °C, 0.5 h, 1M HCl, Aliquat 336, KI, 1-bromobutane, reflux, 12 h (76%); (ii) $NaNO_2$, HNO_3, 0 °C, 1 h (90 %); (iii) triethyl phosphite, 160 °C, reflux, 4 h, N_2, (60%); (iv) NaH, 1-iodoethane, Dry THF, reflux, 17 h (75%); (v) p-toluene sulphonic acid mono hydrate, toluene, 100 °C, 30 h (90%); (vi) 8, zinc acetate, imidazole, 165 °C, microwave, 30 min. (80–90%); (vii) sulfur powder, anh. NMP, N_2, 70 °C, 0.5 h, 180 °C, 17 h (55%); (viii) selenium powder, anh. NMP, N_2, 70 °C, 0.5 h, 180 °C, 17 h (55 %).

Scheme 2. Synthesis of 3,4,5-tris(decyl)aniline



Reagents and conditions. (I) $NaNO_2$, H_2SO_4, AcOH, H_2O, KI, 90 °C, 91% (II) CuI, Et_3N, 4h, $Pd(PPh_3)_2Cl_2$, 80 °C, 4h, 89% (III) EtOAc, MeOH, H_2-Pd/C, rt, overnight, 95%.

Procedure for the synthesis of 3, 4, 5-Triiodonitrobenzene (6): [S1]

An ice-cold solution of sodium nitrite (1.37 g) in concentrated sulfuric acid (7.7 mL) was added dropwise into a well-stirred suspension of 2,6-diiodo-4-nitroaniline (5.5 g, 0.014 mol) in acetic acid (33 mL) in an ice-bath. The reaction mixture was kept below 25 °C with stirring until all diiodonitroaniline was dissolved. The resulting deep yellow solution was poured into ice water (200 mL). Urea (0.5 g) was added into the above reaction solution to remove the excess nitrous acid and then filtered. The filtrate was added with the solution of potassium iodide (3.30 g) in water (16.5 mL) dropwise with vigorous stirring, leading to the formation of a yellow precipitate. The reaction mixture was heated to 85-90 °C in a water-bath, and afterwards cooled to room temperature. Sodium bisulfite (0.5 g) was added into the reaction solution to remove excess iodine. The yellow precipitate was separated by filtration and washed with water, then dried in vacuum. The crude product was purified by silica gel column chromatography with n-hexane /dichloromethane (1:1) as eluent to give a yellow solid. (6.40 g, 91%). R_f = 0.6 (5% EtOAc-Hexane). ^{1}H-NMR (600 MHz, $CDCl_3$, 299 K): δ = 8.61 (s, 2H, Ar-H). ^{13}C NMR (150 MHz, $CDCl_3$, 298.1K): δ 147.50, 132.86, 131.02, 106.96; MALDI-TOF exact mass calculated for $C_6H_2I_3NO_2$ ($M+H^+$): 501.80, found: 501.89.

Procedure for the Synthesis of 3,4,5-Tris(1'-decynyl)-nitrobenzene (7): [S2]

To a well stirred suspension of 3,4,5-Triiodonitrobenzene (3.0 g, 6.0 mmol), bis(triphenylphosphine)-palladium(II) dichloride (252 mg, 0.30 mmol), copper(I) iodide (115 mg, 0.60 mmol) in triethylamine (80 mL) under argon atmosphere at 80 °C, 1-decyne (2.737 g, 19.8 mmol) was added dropwise and the reaction mixture was stirred for another 4 h, maintaining the same conditions. After cooling to room temperature, the solid precipitate was filtered and the filtrate was concentrated by rotary evaporation. The residue was purified by silica gel column chromatography with *n*-hexanes to obtain a brown oil (2.9 g, 89%). R_f =

0.70 (5% EtOAc-Hexane). ^{1}H NMR (600 MHz, $CDCl_3$, 299 K): δ = 8.08 (s, 2H, Ar-H), 2.54-2.46 (t, 6H, *J* = 7.0 Hz, C≡CCH_2), 1.65 (m, 6H, CH_2), 1.4-1.1 (m, 30H, CH_2), 0.88 (t, 9H, *J* = 6.7 Hz, CH_3). MALDI-TOF exact mass calculated for $C_{36}H_{53}NO_2$ ($M+H^+$): 532.83, found: 532.67.

Procedure for the synthesis of 3,4,5-Trisdecylaniline (8): [S2]

1,2,3-Tri(1-decynyl)-5-nitrobenzene (1.5 g, 2.82 mmol) was dissolved in a mixture of ethyl acetate (25 mL) and methanol (5 mL). Argon was bubbled through the solution for 15 minutes after which Pd/C (160 mg) was carefully added and the mixture was subsequently subjected to hydrogenation in a Parr hydrogenation apparatus at 150 psi for 24 h. Upon completion of the reaction, the suspension was filtered and the filtrate was concentrated *in vacuo* to yield a reddish brown viscous liquid (1.38 g, 95%). R_f = 0.3 (5% EtOAc-Hexane). ^{1}H NMR (600MHz, $CDCl_3$, 299 K): δ = 6.38 (s, 2H, Ar-H), 2.47 (t, J = 7.4 Hz, 6H, $ArCH_2$),1.6–1.0 (m, 48H, aliphatic), 0.88 (t, J = 6.8 Hz, 9H, CH_3). MALDI-TOF exact mass calculated for $C_{36}H_{65}NH_2$ ($M+H^+$): 514.94, found: 514.64.

General procedures for synthesis of PBIs [S3]

Compound **1, 2, 3 & 4** (1 eq.), tridecyl aniline (2.2 eq.), zinc acetate (2 eq.) and imidazole (1 g) were taken in a microwave vessel, flushed with nitrogen and put in microwave reactor. The mixture was heated to 165 °C for 35 minutes at 35 W and 100 psi pressure. After cooling, reaction mixture was poured into a 2N HCl (10 mL) solution and extracted with chloroform. Organic layer was washed with water and saturated sodium chloride solution. The crude compound was purified by neutral alumina column chromatography using 50% chloroform-hexane system. Further purification was done by recrystallization from chloroform-methanol system.

PBI[10] : R_f = 0.6 (10% EtoAc-Hexane); Dark red waxy solid, yield: 86%; IR: ν_{max} in cm^{-1}: 2955, 2924, 2854, 1698, 1664, 1592, 1504, 1464, 1439, 1404, 1371, 1332, 1240, 1196, 1114, 858, 809, 744, 722; ^{1}H NMR (600 MHz, $CDCl_3$, 299 K): 8.73 (d, *J* = 12 Hz, 4H, H_{Ar}), 8.63 (d, *J* = 6 Hz, 4H, H_{Ar}), 6.98 (s, 4H, H_{Ar}), 2.65 (t, 12H, 6 × -CH_2), 1.6 (m, 12H, 6 × -CH_2), 1.5-1.1 (m, 84H, 42 × -CH_2), 0.88 (t, 18H, 6 × -CH_3); ^{13}C NMR (150 MHz, $CDCl_3$, 298.1 K): δ 163.85, 142.41, 139.52, 134.99, 132.34, 131.91, 129.87, 126.78, 126.40, 123.84, 123.41, 77.44, 77.33, 77.02, 33.39, 32.18, 32.14, 31.50, 30.98, 30.67, 30.25, 29.92, 29.88, 29.86, 29.74, 29.66, 29.64, 22.59, 22.91, 14.37, 14.35; MALDI-TOF exact mass calculated for $C_{96}H_{138}N_2O_4$ $(M)^-$: 1384.09, found: 1384.031.

PBI-N[10] : R_f = 0.6 (10% EtOAc-Hexane); Dark red waxy solid, yield: 86%; IR: ν_{max} in cm^{-1} :2955, 2923, 2854, 1706, 1667, 1595, 1561, 1466, 1427, 1364, 1351, 1319, 1244, 1185,1127, 845, 807, 744, 722; ^{1}H NMR (600 MHz, $CDCl_3$, 299 K): 9.03 (s, 2H, H_{Ar}), 8.94 (d, *J* =12Hz, 2H, H_{Ar}), 8.87 (d, *J* =12 Hz, 2H, H_{Ar}),7.06 (s, 4H, H_{Ar}), 4.98 (d, *J* = 6 Hz, 2H, N-$\underline{CH_2}$) 2.69 (t, 12H, 6 × -CH_2), 1.66 (t, 3H, N-CH_2-$\underline{CH_3}$), 1.58 (m, 12H, 6 × -CH_2), 1.42-1.26 (m, 84H, 42 × -CH_2), 0.88 (t, 18H, -CH_3); ^{13}C NMR (150 MHz, $CDCl_3$, 298.1 K): δ 165.67, 164.54, 142.47, 139.57, 134.63, 133.87, 132.76, 130.25, 128.20, 126.69,124.06, 123.14, 122.99, 120.16, 119.21, 41.96, 32.17, 30.29, 30.24, 29.92, 29.79, 29.75, 29.71, 29.68, 29.60, 22.94, 22.90, 17.07, 14.38, 14.34; MALDI-TOF exact mass calculated for $C_{98}H_{141}N_3O_4$ $(M)^-$: 1425.11, found: 1425.049.

PBI-S[10] : R_f = 0.6 (10% EtoAc-Hexane); Orange red waxy solid, yield: 78%; IR: ν_{max} in cm^{-1} :2955, 2923, 2854, 1706, 1667, 1595, 1561, 1466, 1427, 1364, 1351, 1319, 1244, 1185,1127, 845, 807, 744, 722; ^{1}H NMR (600 MHz, $CDCl_3$, 299 K): 9.39 (s, 2H, H_{Ar}), 9.03 (d, *J* = 12 Hz, 2H, H_{Ar}), 8.99 (d, *J* =12 Hz, 2H, H_{Ar}),7.03 (s, 4H, H_{Ar}), 2.67 (t, 12H, 6 × -CH_2), 1.6 (m, 12H, 6 × -CH_2), 1.5-1.1 (m, 84H, 42 × -CH_2), 0.88 (t, 18H, 6 × -CH_3); ^{13}C NMR (150 MHz, $CDCl_3$, 298.1 K): δ 164.54, 164.09, 142.48, 139.57, 138.63, 133.87, 132.76, 132.13, 130.25, 128.20, 126.69, 126.50, 124.06, 123.73, 123.38, 122.99, 33.40, 32.17, 32.13, 31.50, 30.97, 30.68, 30.24, 29.92, 29.88, 29.86, 29.75, 29.66, 29.64, 29.59, 29.05, 22.94, 22.90, 14.38, 14.34; MALDI-TOF exact mass calculated for $C_{96}H_{136}N_2O_4S(M)^-$: 1414.802, found: 1414.509.

PBI-Se[10] : R_f = 0.6 (10% EtoAc-Hexane); Dark red waxy solid, yield: 76%; IR: ν_{max} in cm^{-1} :2955, 2923, 2854, 1706, 1667, 1595, 1561, 1466, 1427, 1364, 1351, 1319, 1244, 1185, 1127, 845, 807, 744, 722; ^{1}H NMR (600 MHz, $CDCl_3$, 299 K): 9.37 (s, 2H, H_{Ar}), 8.94 (d, *J* =12 Hz, 2H, H_{Ar}), 8.92 (d, *J* =12 Hz, 2H, H_{Ar}), 7.03 (s, 4H, H_{Ar}), 2.67 (t, 12H, 6 × -CH_2), 1.6 (m, 12H, 6 × -CH_2), 1.5-1.1 (m, 84H, 42 × -CH_2), 0.88 (t, 18H, 6 × -CH_3); ^{13}C NMR (150 MHz, $CDCl_3$, 298.1 K): δ 164.54, 164.05, 142.46, 140.99, 138.63, 139.53, 134.88, 133.95, 132.69, 130.50, 126.50, 124.95, 123.55, 123.08, 122.53, 33.40, 32.18, 32.14, 31.49, 30.99, 30.69, 30.26, 29.93, 29.88, 29.87, 29.75, 29.67, 29.65, 29.59, 29.05, 22.95, 22.91, 14.38, 14.35; MALDI-TOF exact mass calculated for $C_{96}H_{136}N_2O_4Se(M)^-$: 1461.13, found: 1461.935.

3. NMR Spectra

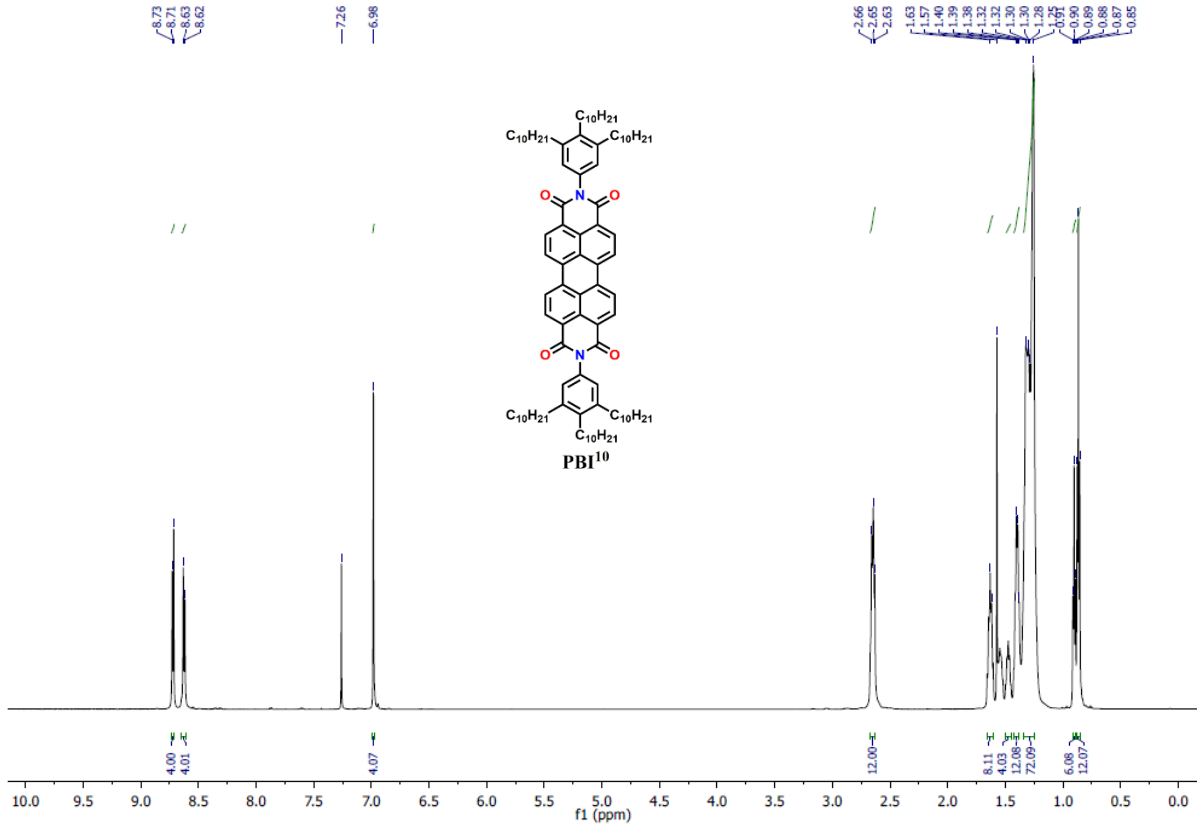


Figure S1. ^{1}H NMR (600 MHz) spectra of **PBI^{10}** in $CDCl_3$.

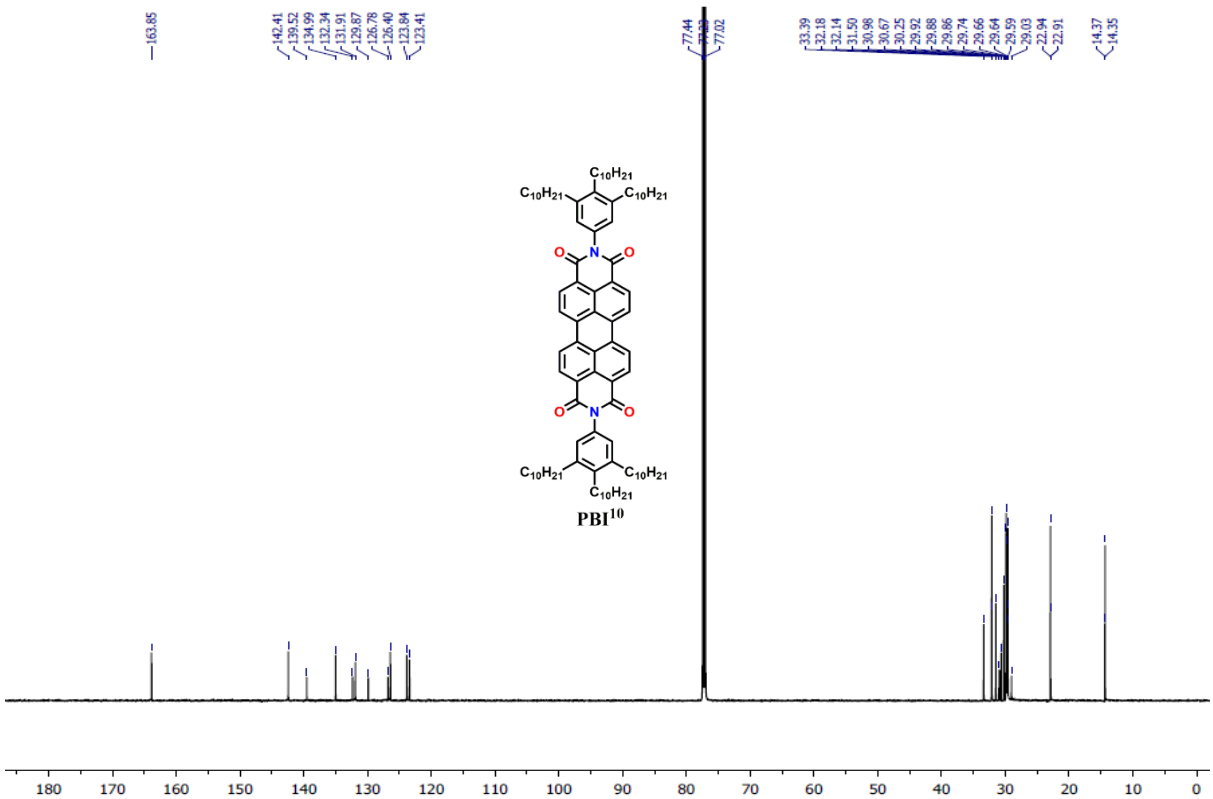


Figure S2. ^{13}C NMR (150 MHz) spectra of **PBI^{10}** in $CDCl_3$.

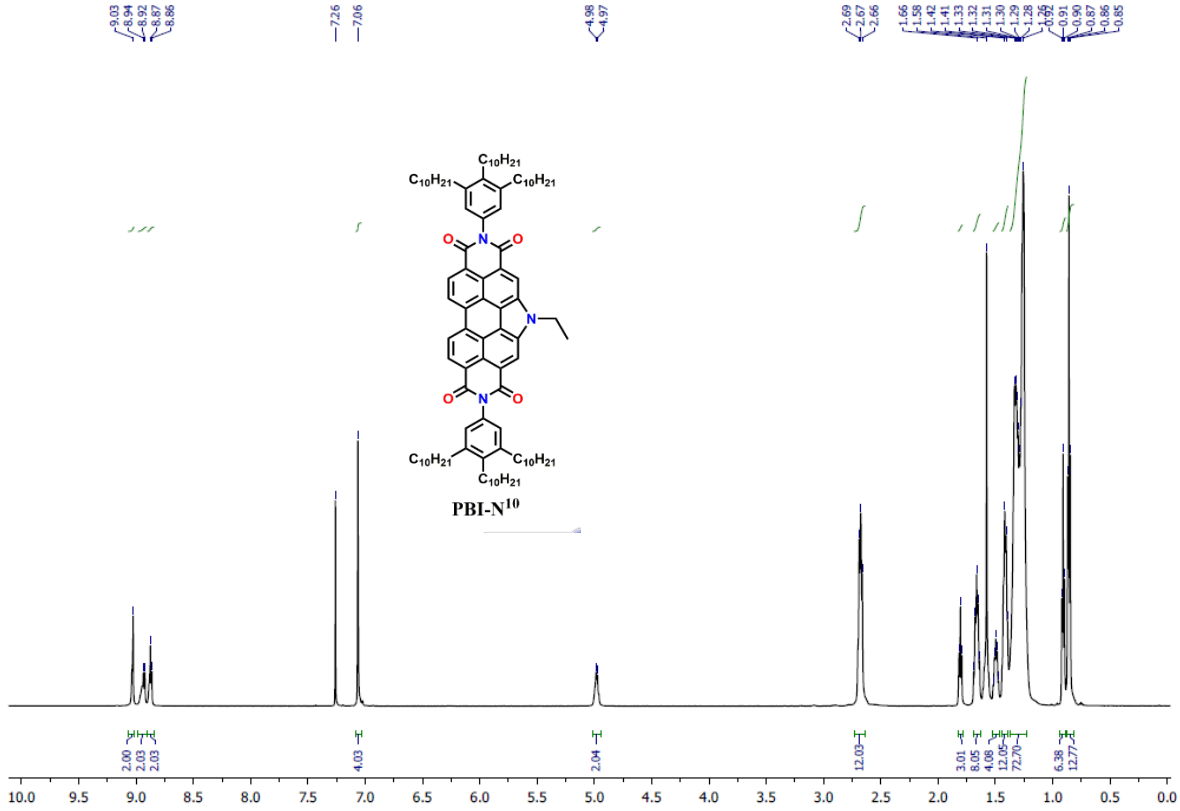


Figure S3. ^{1}H NMR (600 MHz) spectra of **PBI-N^{10}** in $CDCl_3$.

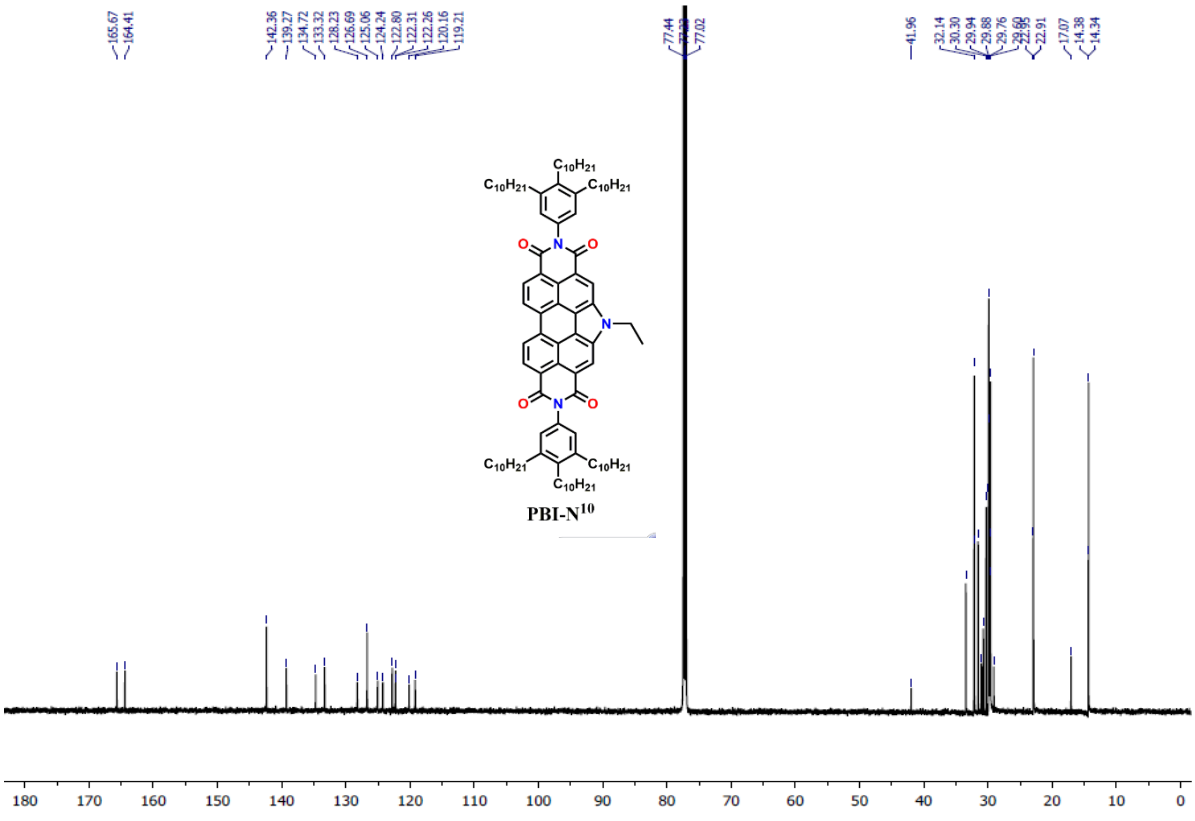


Figure S4. ^{13}C NMR (150 MHz) spectra of **PBI-N^{10}** in $CDCl_3$.

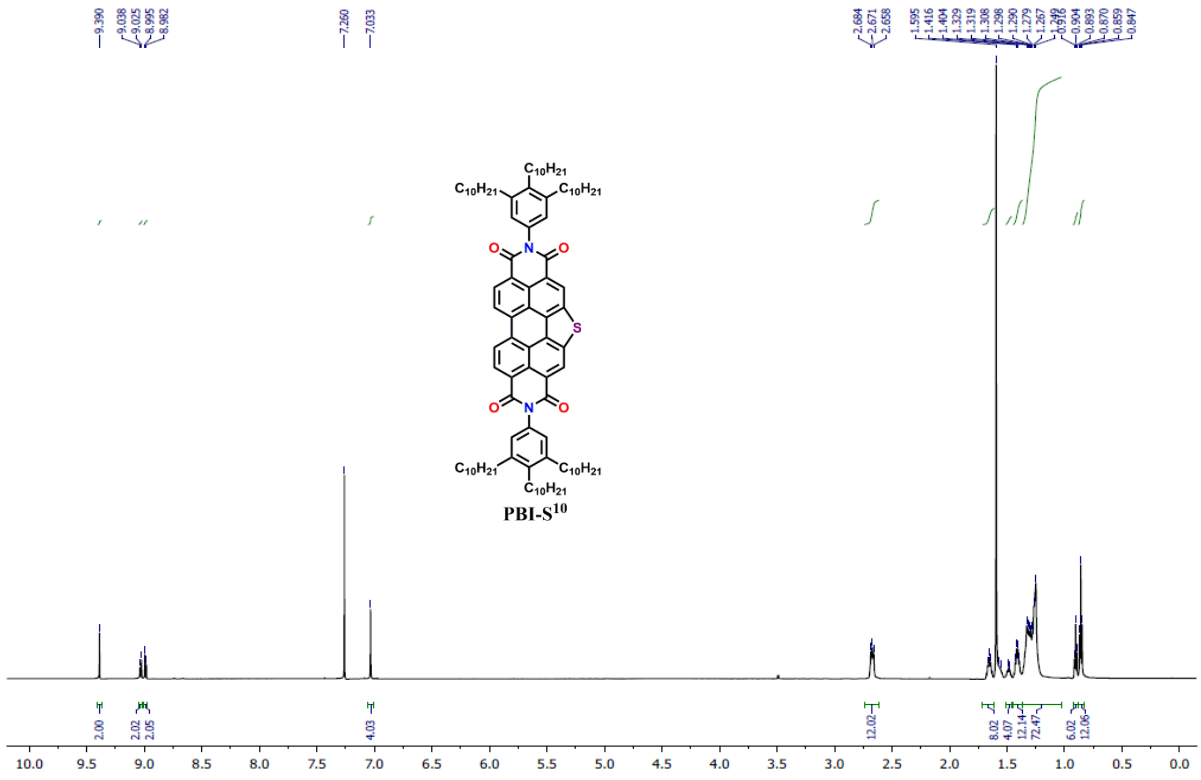


Figure S5. ^{1}H NMR (600 MHz) spectra of **PBI-S^{10}** in $CDCl_3$.

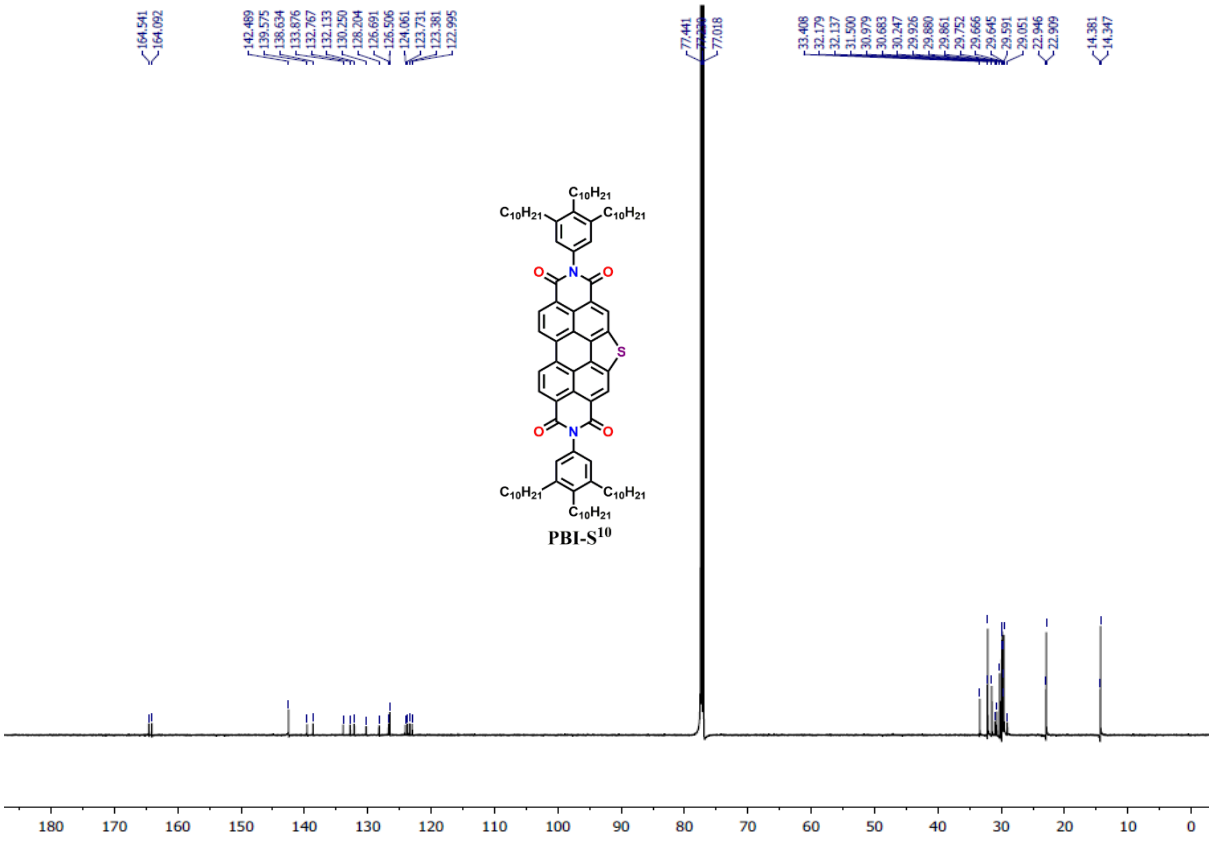


Figure S6. ^{13}C NMR (150 MHz) spectra of **PBI-S^{10}** in $CDCl_3$.

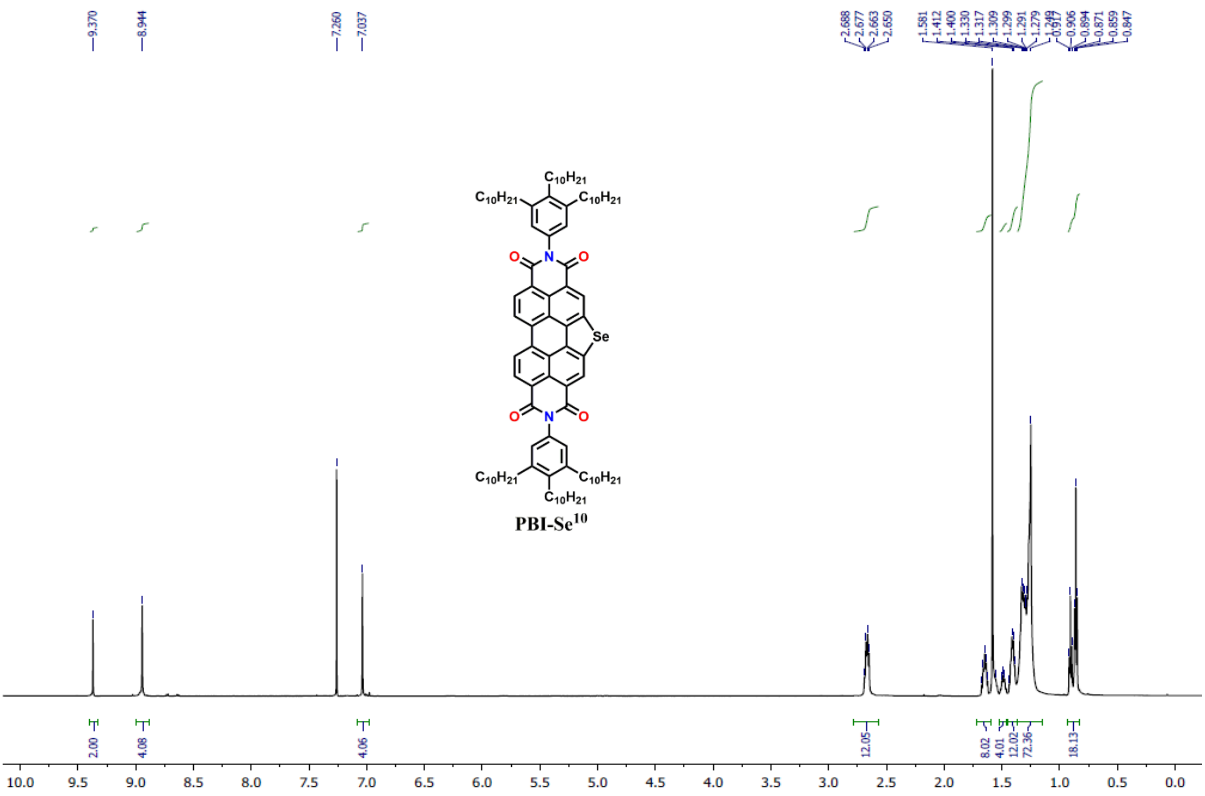


Figure S7. ^{1}H NMR (600 MHz) spectra of **PBI-Se^{10}** in $CDCl_3$.

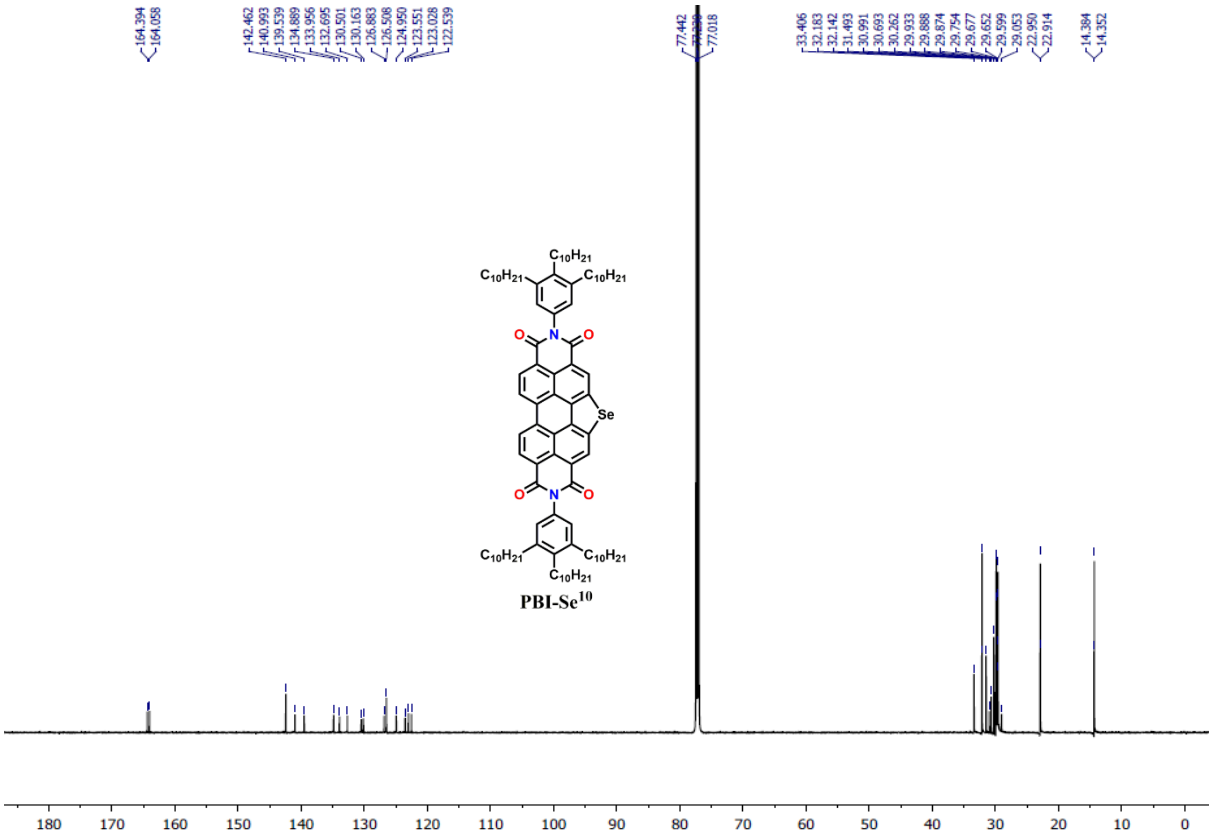


Figure S8. ^{13}C NMR (150 MHz) spectra of **PBI-Se^{10}** in $CDCl_3$.

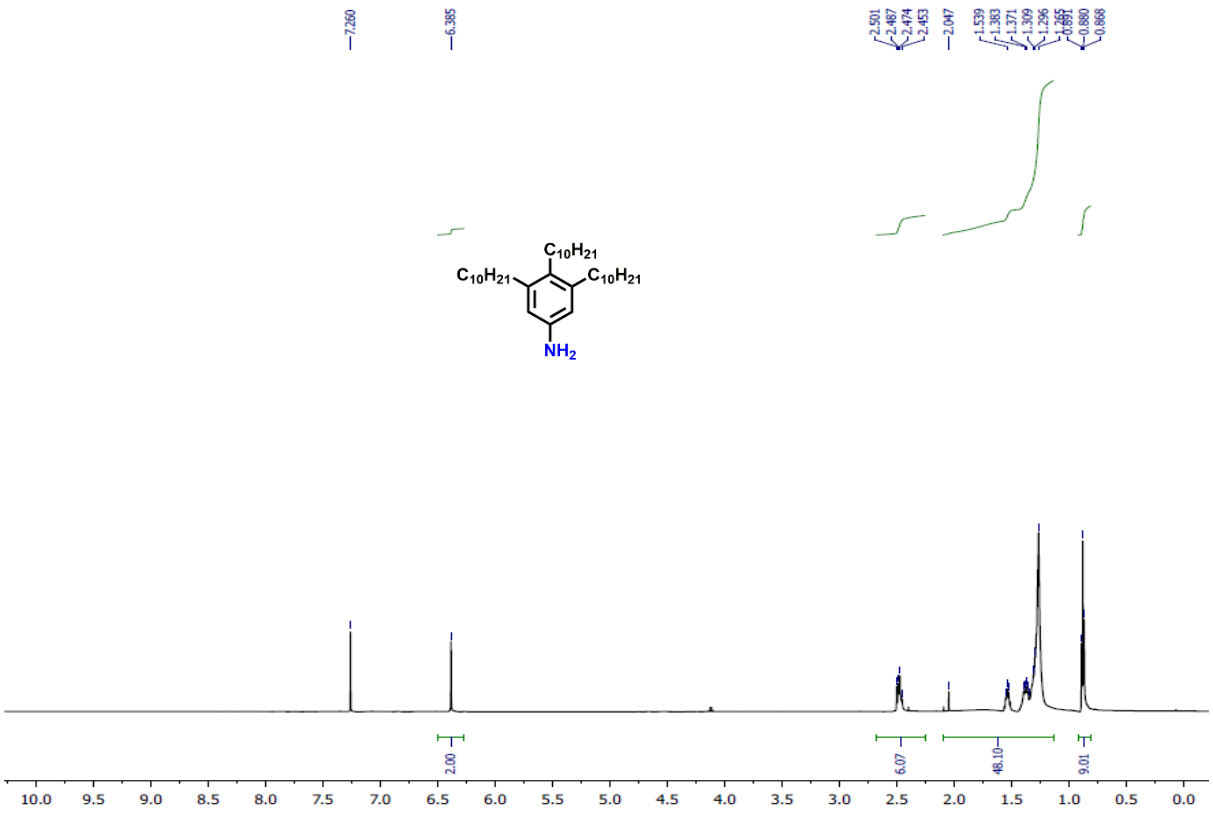


Figure S9. ^{1}H NMR (600 MHz) spectra of 3,4,5-Trisdecylaniline **(8)** in $CDCl_3$.

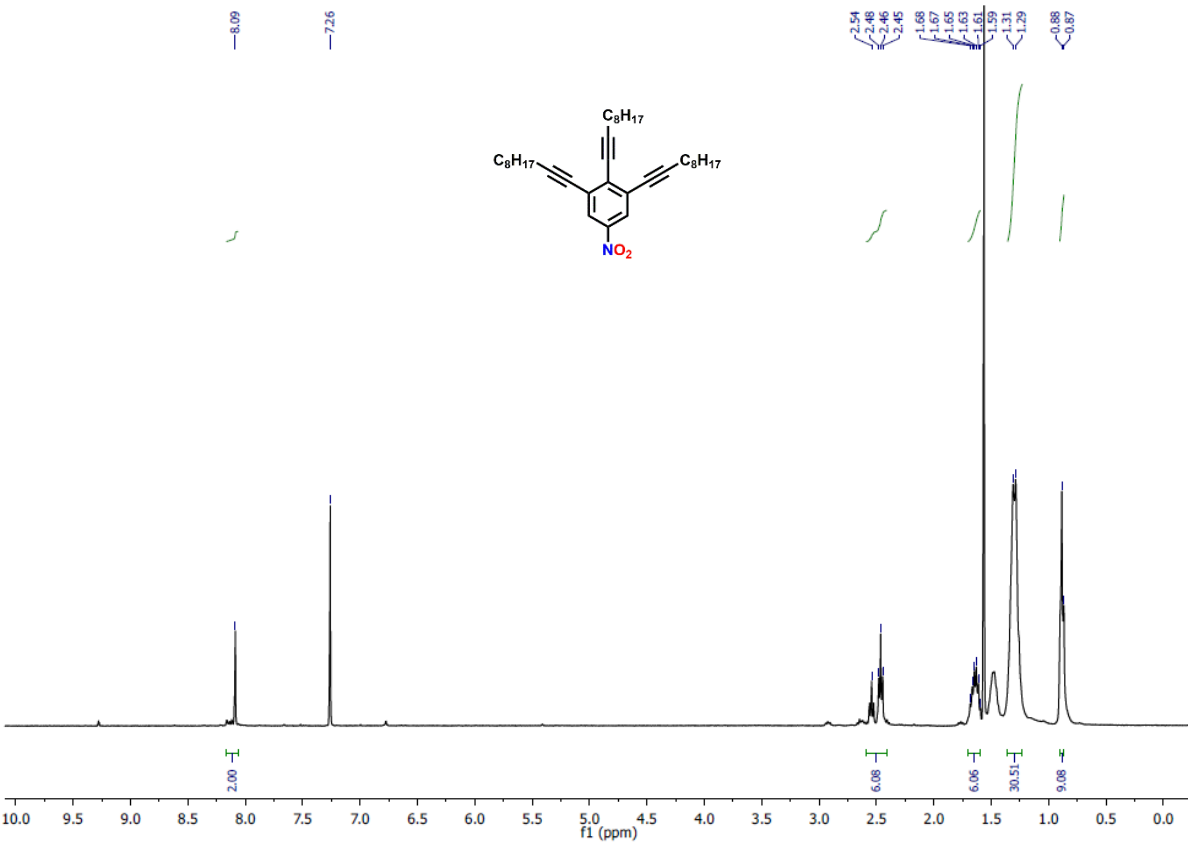


Figure S10. ^{1}H NMR (600 MHz) spectra of 3,4,5-Tris(1'-decynyl)-nitrobenzene **(7)** in $CDCl_3$.

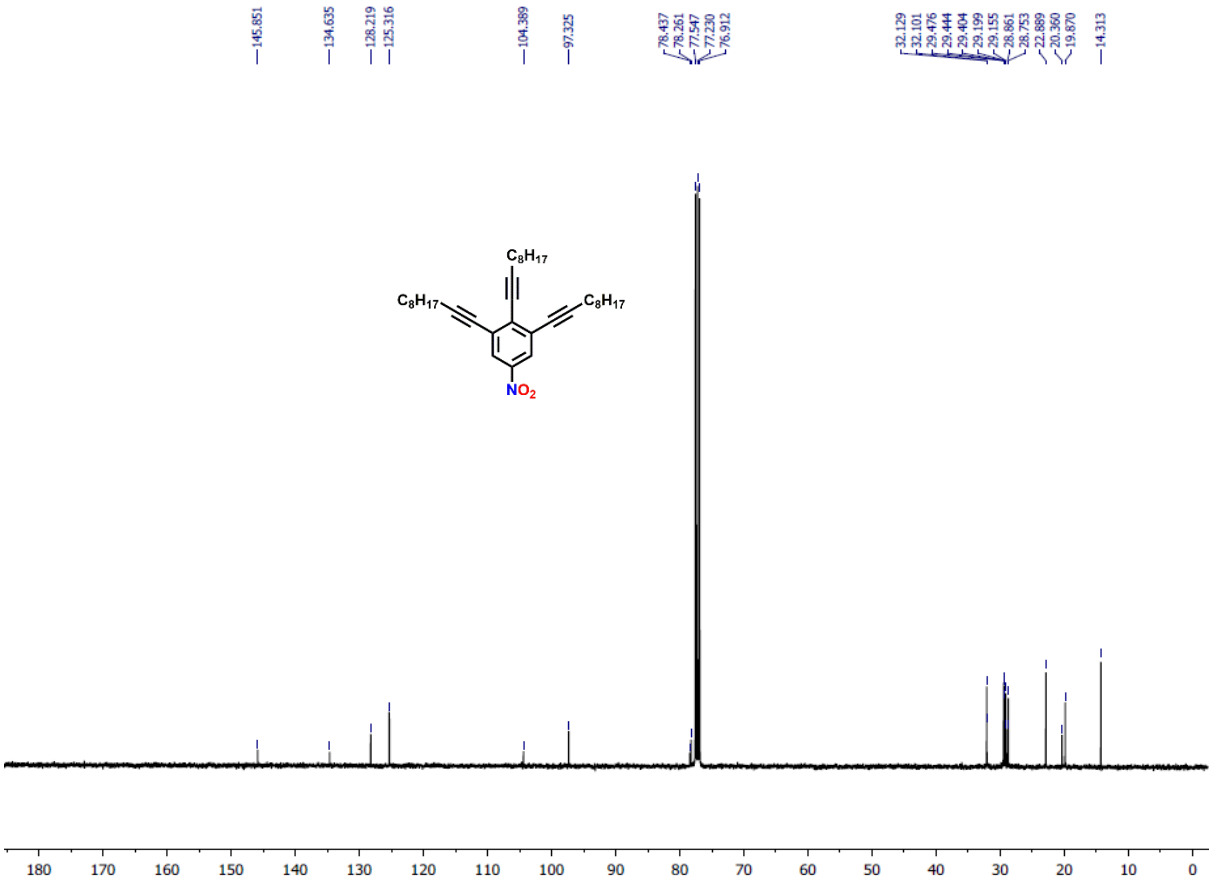


Figure S11. ^{13}C NMR (150 MHz) spectra of 3,4,5-Tris(1'-decynyl)-nitrobenzene **(7)** in $CDCl_3$.

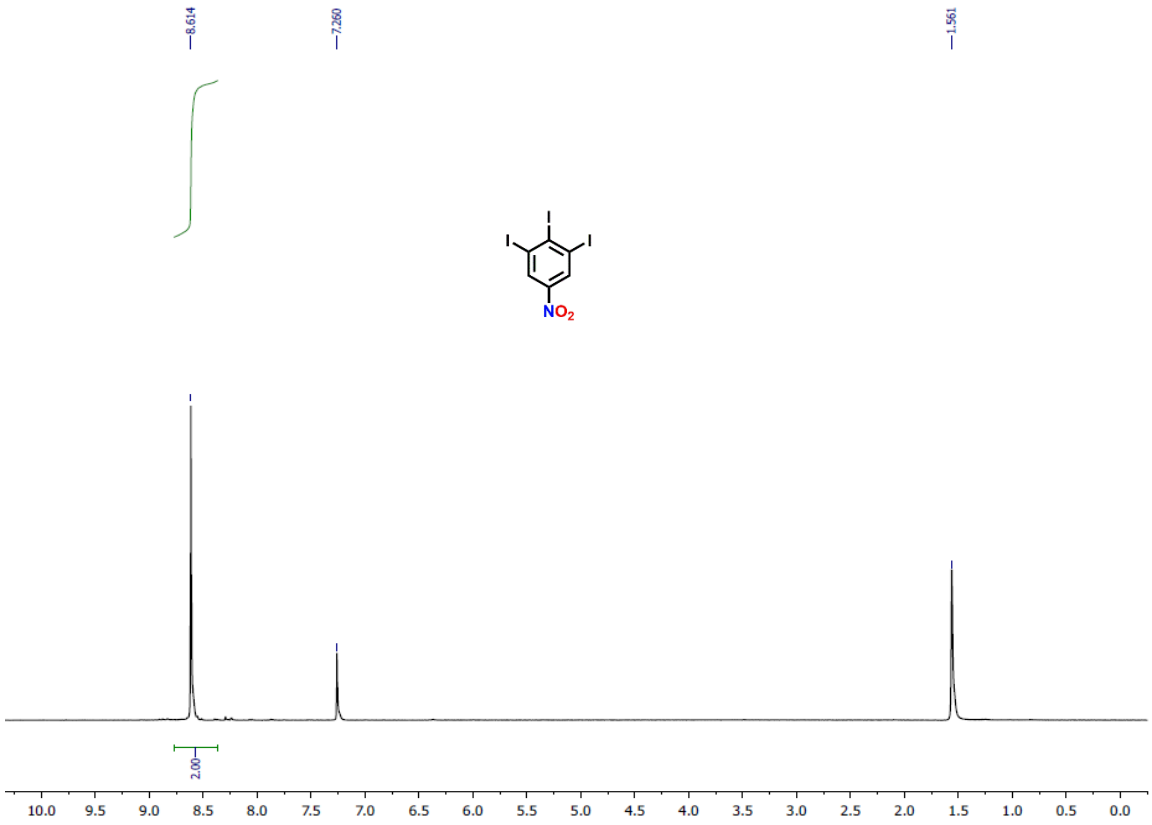


Figure S12. ^{1}H NMR (600 MHz) spectra of 3, 4, 5-Triiodonitrobenzene **(6)** in $CDCl_3$.

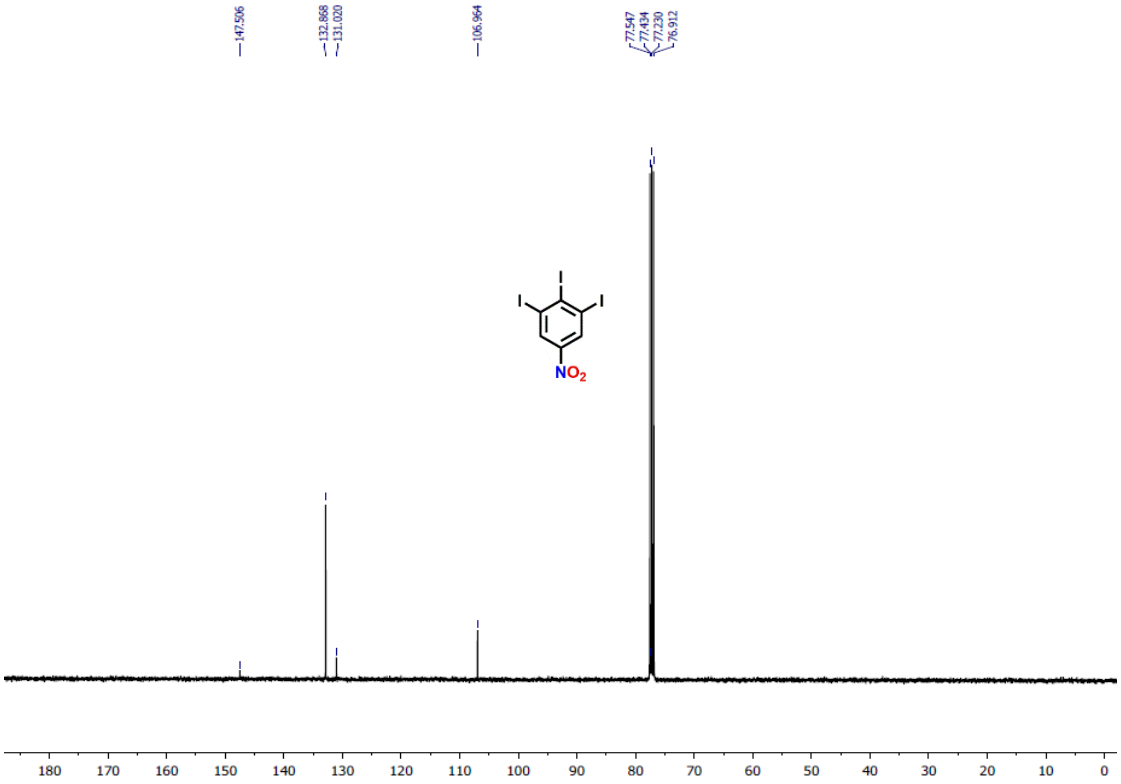


Figure S13. ^{13}C NMR (150 MHz) spectra of 3, 4, 5-Triiodonitrobenzene **(6)** in $CDCl_3$.

4. MALDI-TOF mass spectra

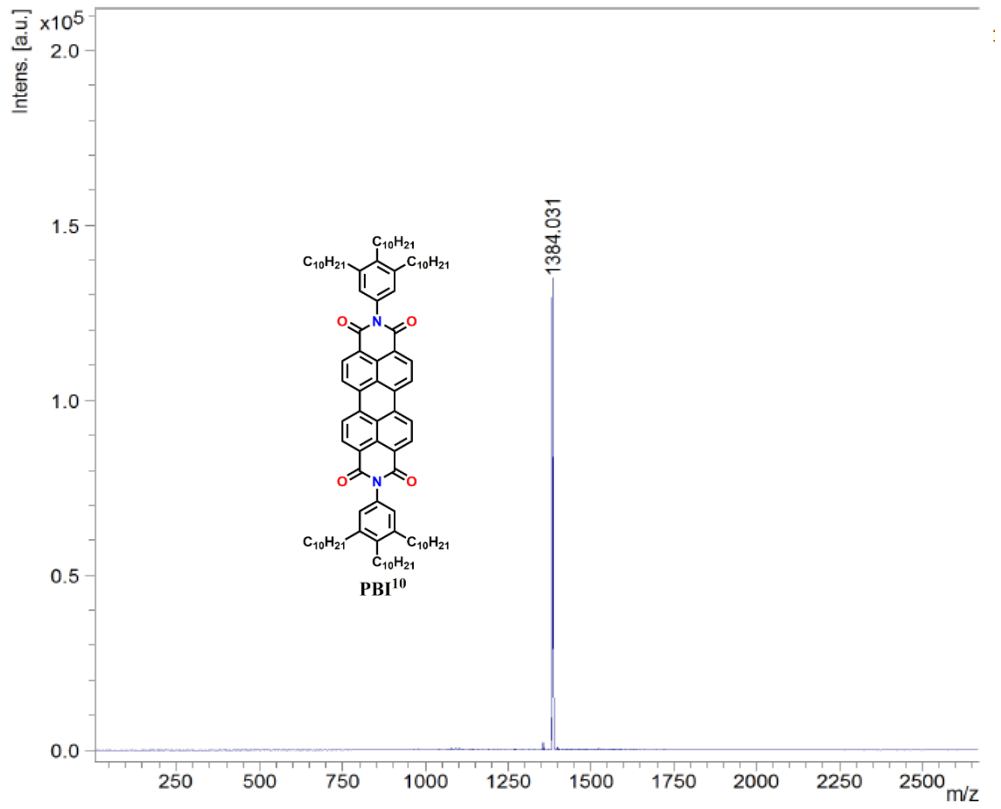


Figure S14. MALDI-TOF mass spectrum of **PBI[10].**

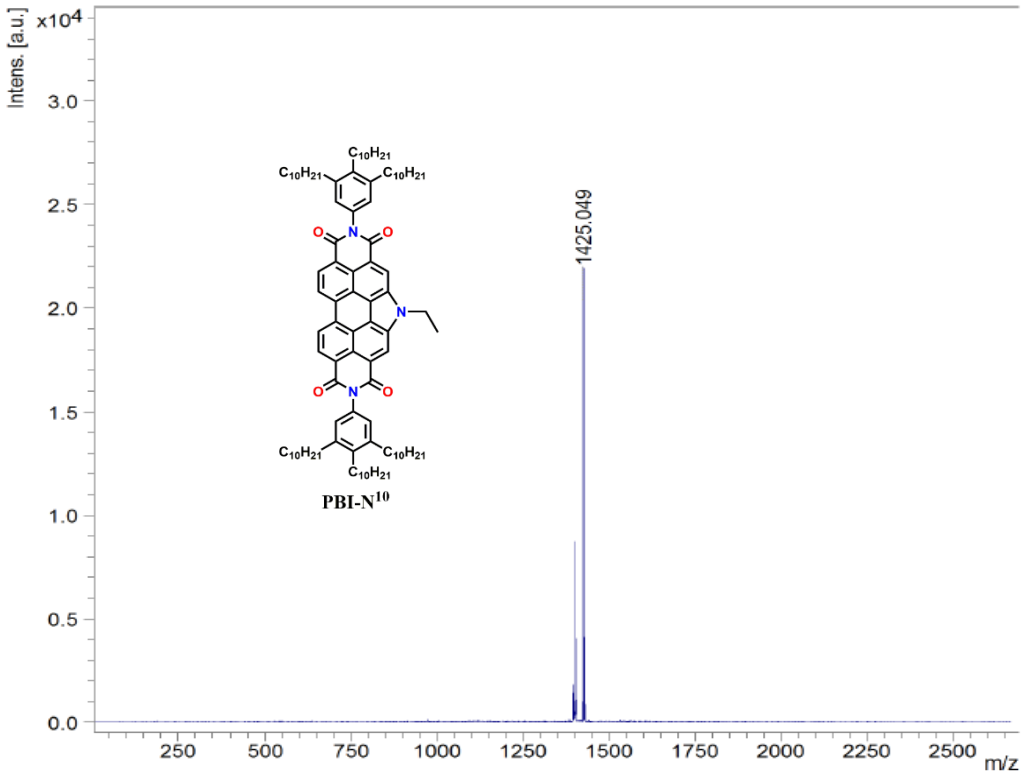


Figure S15. MALDI-TOF mass spectrum of **PBI-N[10]**.

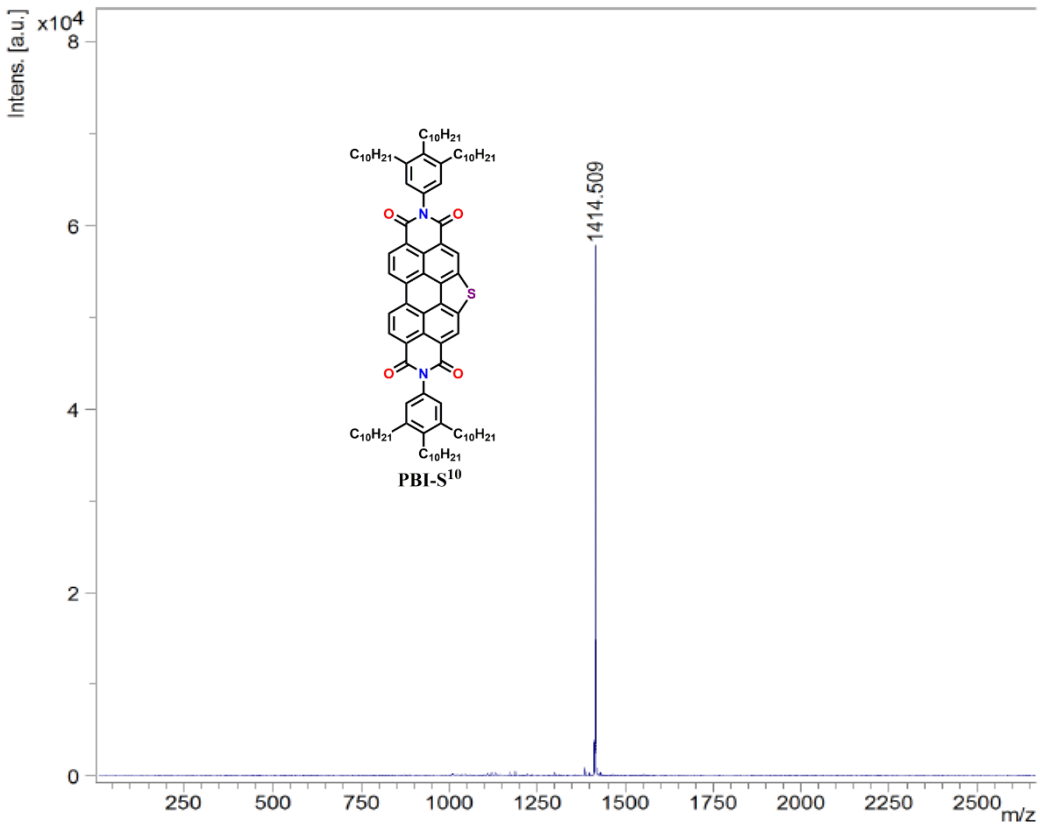


Figure S16. MALDI-TOF mass spectrum of **PBI-S[10]**.

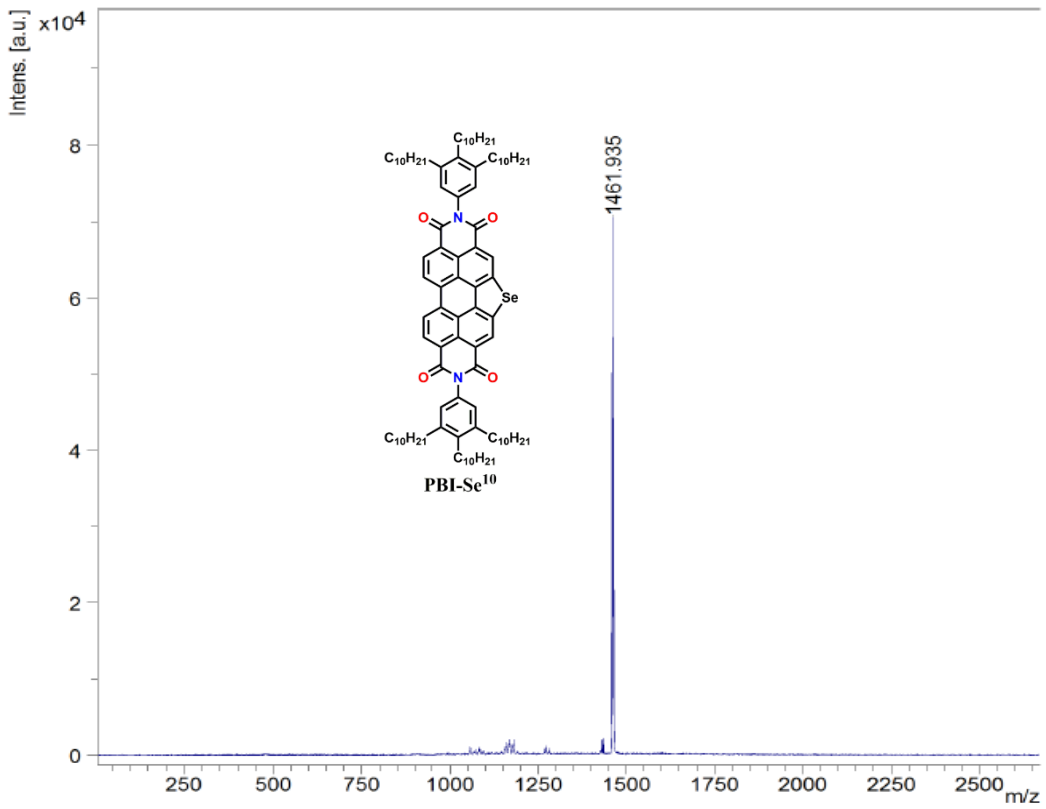


Figure S17. MALDI-TOF mass spectrum of **PBI-Se^{10}**.

5. Photophysical studies

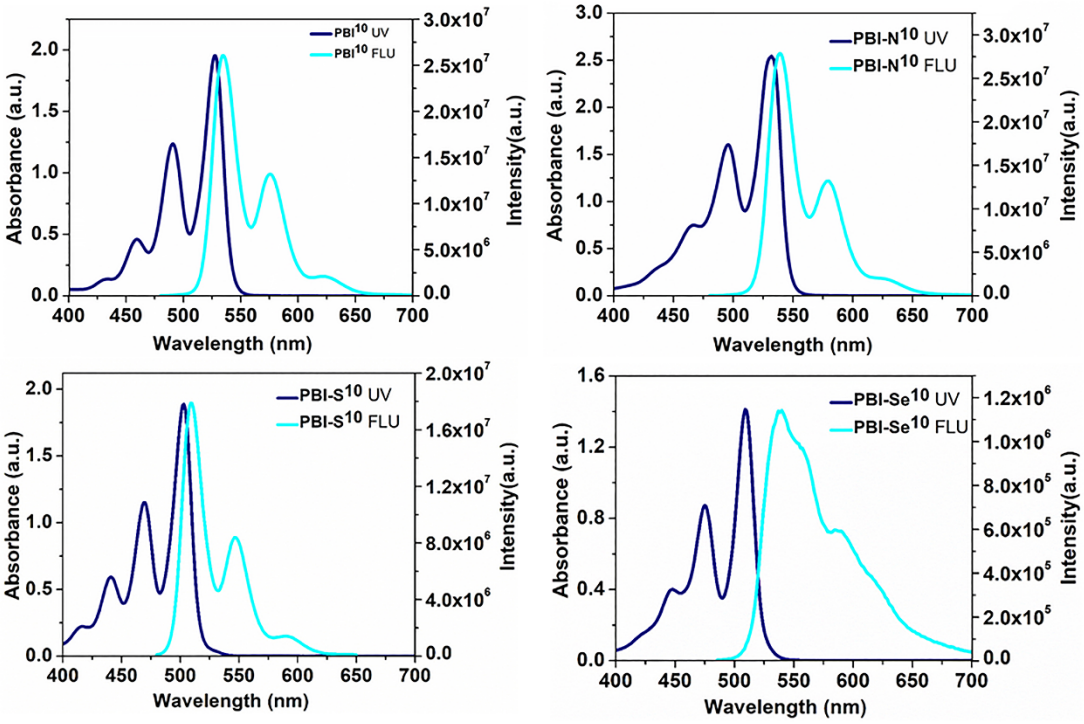


Figure S18. Overlay of absorption (blue trace) and emission (cyan trace) spectra of PBIs in micromolar chloroform solutions.

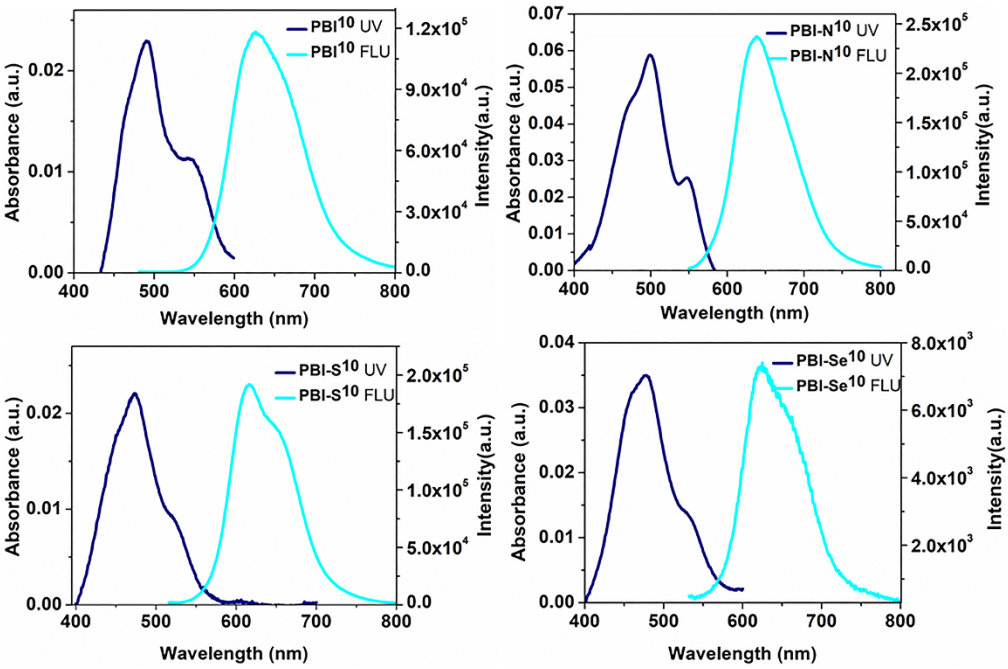


Figure S19. Overlay of absorption (blue trace) and emission (cyan trace) spectra of PBIs in thin film state.

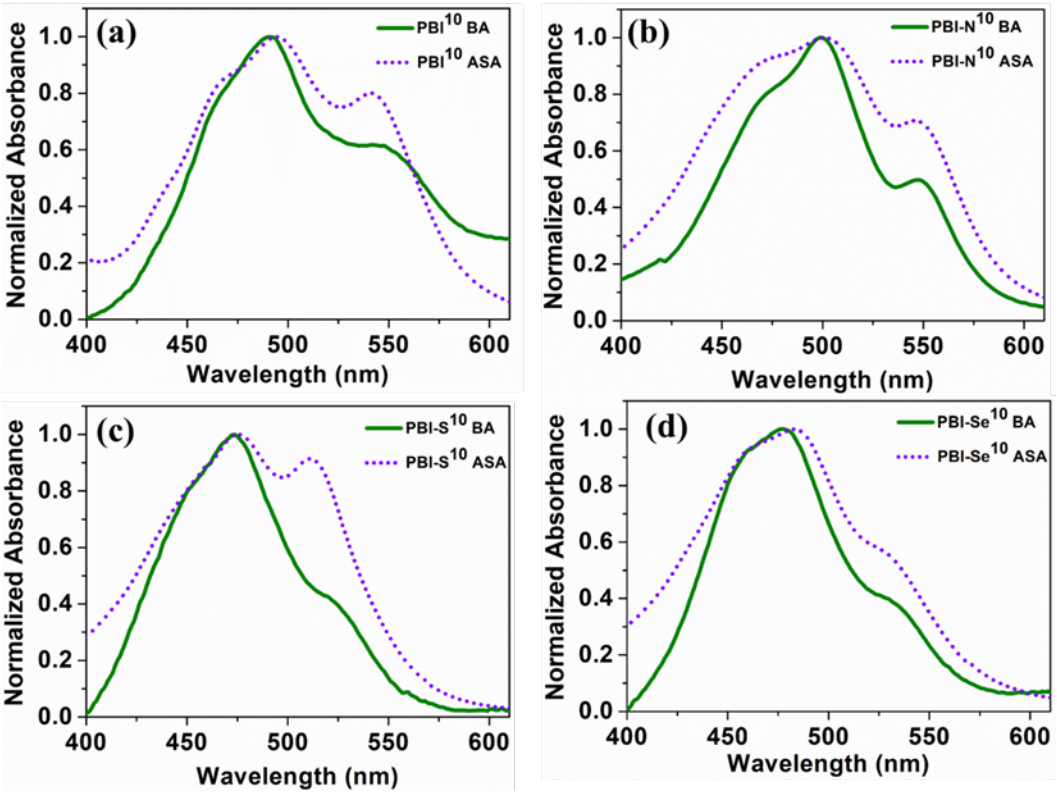


Figure S20. Overlay of the absorption spectra of drop casted thin films of PBIs before (solid line) and after (dotted line) solvent annealing.

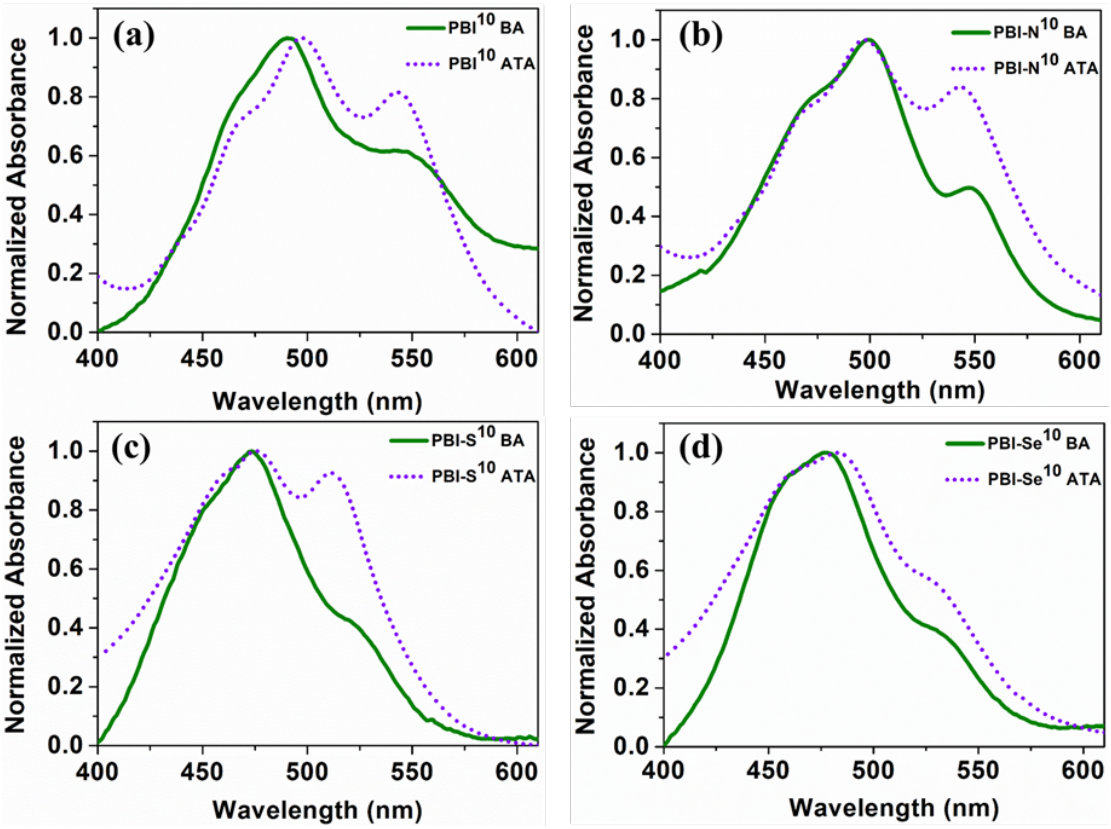


Figure S21. Overlay of the absorption spectra of drop casted thin films of PBIs before (solid line) and after (dotted line) thermal annealing.

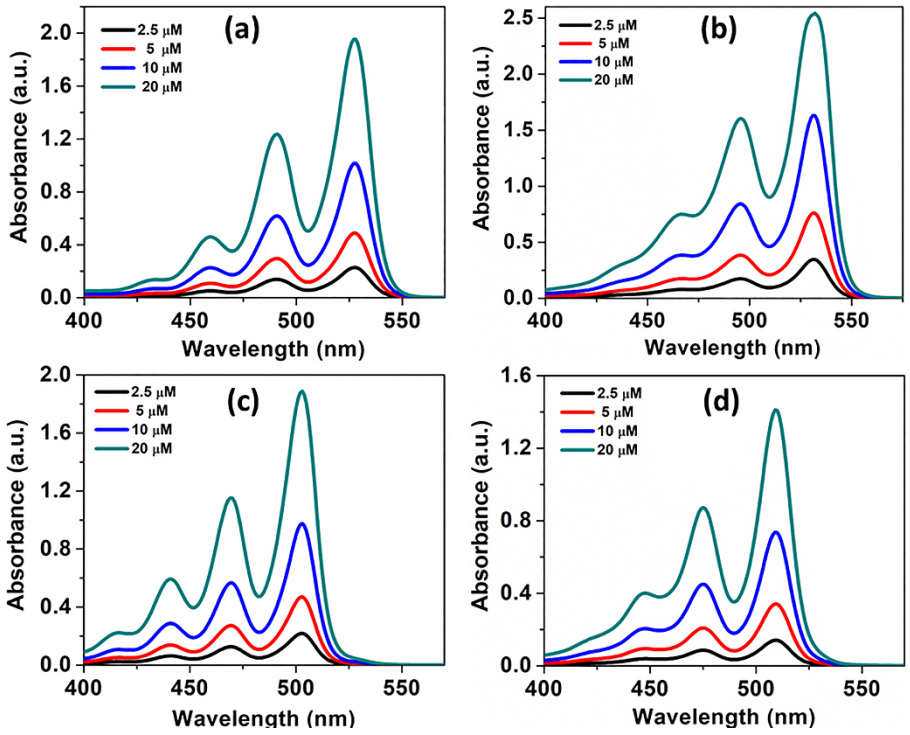


Figure S22. Absorption spectra of **PBI**[10] (a), **PBI-N**[10] (b), **PBI-S**[10] (c) and **PBI-Se**[10] (d) in chloroform solution as a function of concentration.

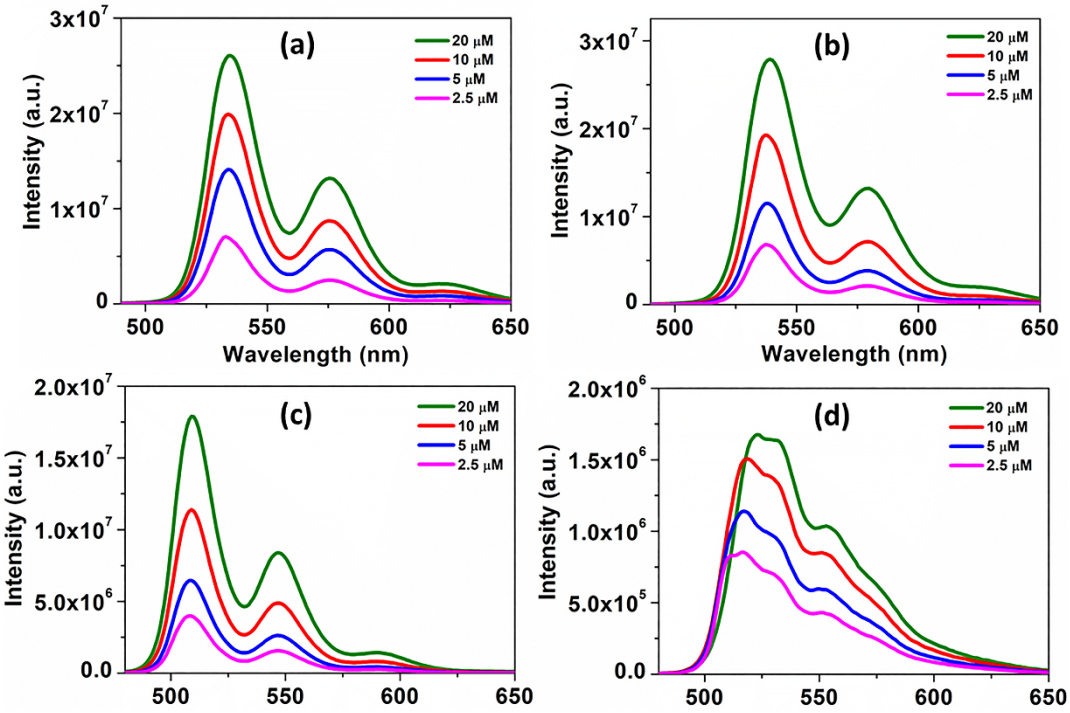


Figure S23. Emission Spectra of **PBI**[10] (a), **PBI-N**[10] (b), **PBI-S**[10] (c) and **PBI-Se**[10] (d) in chloroform solution as a function of concentration.

6. Quantum yield measurement (Relative)

Quantum yield was measured according to established procedure by using rhodamine 6g in ethanol as the standard. Absolute values were calculated according to the following equation: $Q_S = Q_R \times (m_S / m_R) \times (n_S / n_R)^2$, Where, Q: Quantum yield, m: Slope of the plot of integrated fluorescence intensity vs absorbance (Calculated from Fig.S22), n: refractive index (1.361 for ethanol and 1.001 for chloroform). The subscript R refers to the reference fluorophore i.e. rhodamine 6G solution in EtOH and subscript S refers to the sample under investigation. In order to minimize re-absorption effects, absorbance was kept below 0.15 at the excitation wavelength of 527, 532, 503 and 509 nm respectively for compounds PBI[10], PBI-N[10], PBI-S[10] and PBI-Se[10]. Quantum Yield of rhodamine 6g in EtOH is 0.95. Simplified equation for the calculation after substituting the appropriate values is given below and values obtained are given in table below.

$$Q_S = 0.95 \times (m_S / m_R) \times (1.001/1.361)^2$$
$$= 0.513 \times (m_S / m_R)$$

Compounds	$\mathbf{m_S}$	$\mathbf{m_R}$	$\mathbf{Q_S}^{a,b,c}$
PBI[10]	8.44794×10^8	1.4208×10^9	0.62
PBI-N[10]	1.26959×10^{10}	1.5694×10^{10}	0.86
PBI-S[10]	5.10306×10^8	1.3867×10^9	0.39
PBI-Se[10]	2.73086×10^7	1.3942×10^9	0.02

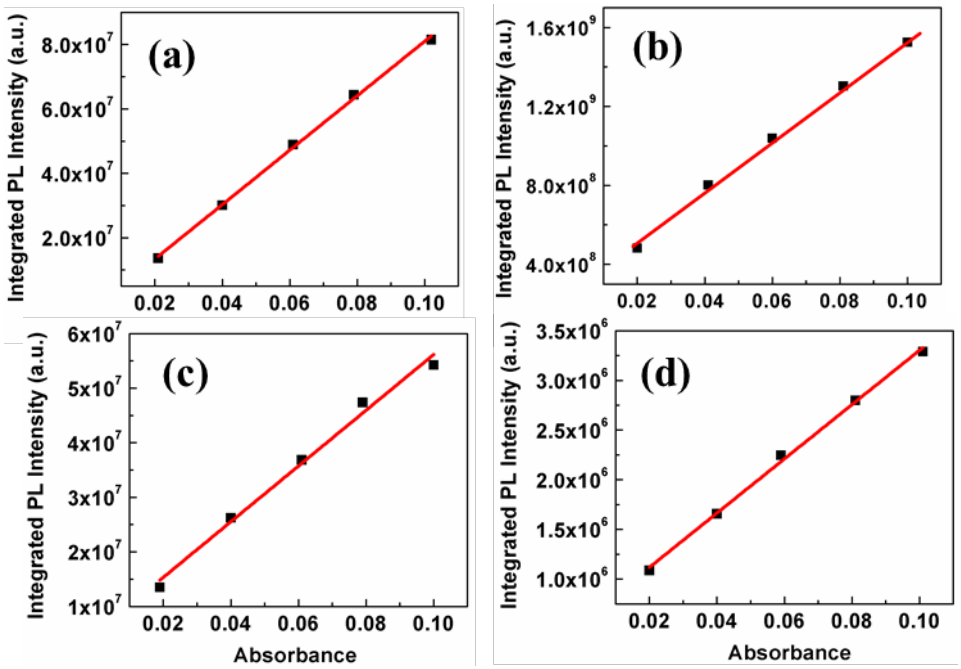


Figure S24. Plots of integrated photoluminescence intensity vs absorbance of reference compound **PBI**[10] (a), **PBI-N**[10] (b), **PBI-S**[10] (c) and **PBI-Se**[10] (d) respectively.

7. Time resolved photoluminescence studies

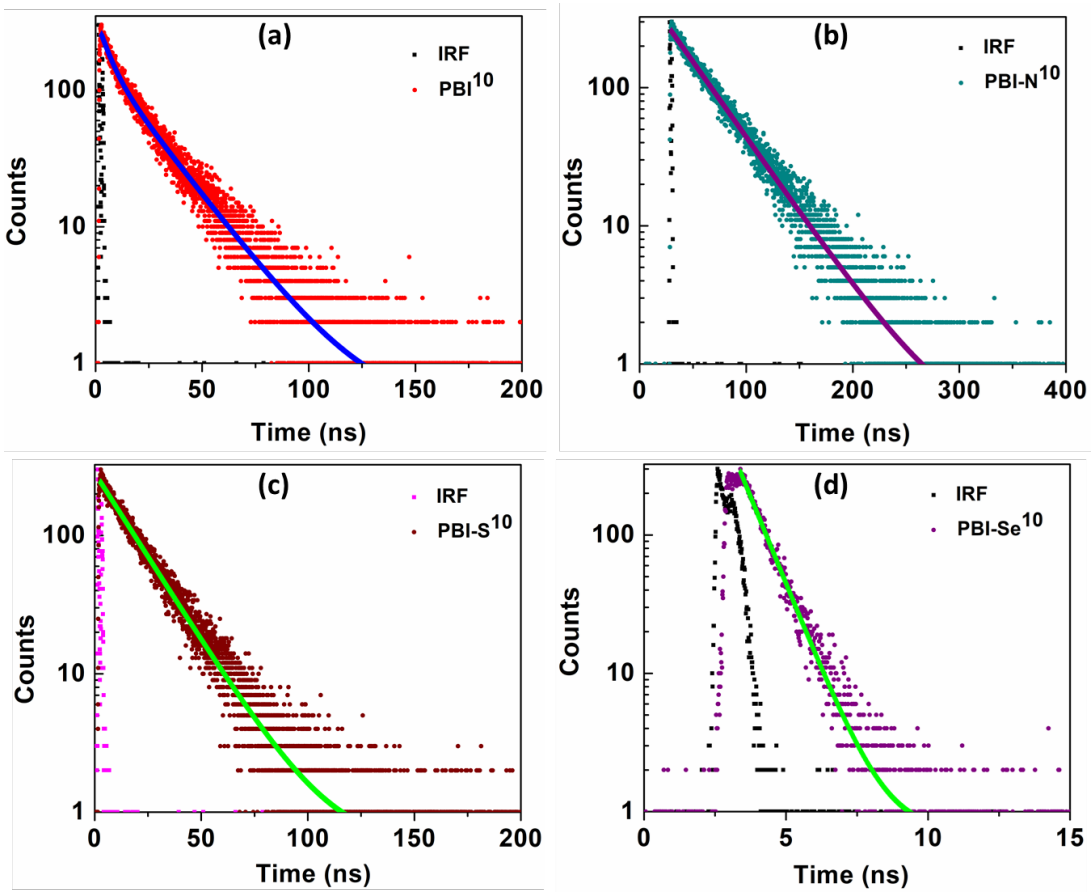


Figure S25. Fluorescence decay plots of compounds **PBI**[10] (a), **PBI-N**[10] (b), **PBI-S**[10] (c) and **PBI-Se**[10] (d) respectively. (IRF: Instrument response function).

Table S1. Data obtained from the time resolved photoluminescence experiments of compounds **PBI**[10], **PBI-N**[10], **PBI-S**[10] and **PBI-Se**[10] respectively.

Sl no.	Compound	τ_1 (ns)
1	**PBI**[10]	17.701
2	**PBI-N**[10]	39.693
3	**PBI-S**[10]	17.850
4	**PBI-Se**[10]	0.859

8. Thermal behavior

Table S2. Phase transition temperatures (^{o}C), corresponding enthalpies (kJmol^{-1})[a] and decomposition temperatures obtained by TGA.

Compounds	Phase Sequence (kJ/mol)		
	Second heating	First Cooling	Temperature at which 5 wt% decomposition occurred (^{o}C)
PBI[10]	Col_h 327.66 (7.82) I	I 323.40 (7.84) Col_h	346
PBI-N[10]	Col_h 338.86 (6.12) I	I 334.32 (5.63) Col_h	356
PBI-S[10]	Col_{ob} 349.23 (4.67) I	I 346.00 (3.67) Col_{ob}	349
PBI-Se[10]	Col_h 343.63 (4.02) I	I 334.76 (3.50) Col_h	348
[a] Peak temperatures in the DSC thermograms obtained during the second heating and first cooling cycles at 5 ^{o}C min^{-1}. Col_h = Columnar hexagonal phase; Col_{ob} = Columnar oblique phase; I = Isotropic phase.			

9. XRD Studies

Table S3. Results of (*hkl*) indexation of XRD profiles of the compounds at a given temperature (T) of mesophases[a]

Compounds (D/Å)	Phase (T/^{o}C)	d_{obs} (Å)	d_{cal} (Å)	Miller indices *hk*	Lattice parameters (Å), Lattice area S (Å^2), Molecular volume (Å^3)
PBI[10] (44.8) MW: 1384.17	Col_h (200)	28.11 16.16 14.64 4.85 (h_a)	28.11 16.23 14.06	10 11 20	a = 32.46
	Col_h (100)	27.74 16.33 13.90 4.65 (h_a) 4.12 (h_c)	27.74 16.02 13.87	10 11 20	a = 32.03
	Col_h (28)	27.44 15.79 13.71 4.60 (h_a) 4.12 (h_c)	27.43 15.84 13.72	10 11 20	a = 31.68 S = 869.2 V = 3584
PBI-N[10]	Col_h	25.98	25.98	10	a = 29.99

(44.6) MW: 1425.22	(200)	14.94 13.21 5.68(h_a) 4.87 (h_c) 3.67 3.41	15.00 12.99 -- -- 3.71 3.33	11 20 53 54	
	Col_h (100)	25.53 14.58 13.11 5.19(h_a) 4.63 (h_c) 3.66 3.38	25.53 14.74 12.76 - - 3.63 3.22	10 11 20 -- -- 44 54	a = 29.48
	Col_h (25)	25.18 14.06 12.63 4.90 (h_a) 4.52 (h_c) 3.64 3.36	25.18 14.54 12.59 3.63 3.22	10 11 20 -- -- 44 54	a = 29.08 S = 732.4 V = 3307.6
PBI-S[10] (43.9) MW: 1414.21	Col_{ob} (200)	28.28 16.32 14.04 9.20 8.36 7.99 4.75 (h_a) 3.99 (h_c)	28.28 16.32 14.14 9.23 8.16 7.87	10 11 02 30 22 13	a = 31.39 b = 32.04 γ = 61.95°
	Col_{ob} (100)	27.67 26.18 15.96 15.03 13.57 4.63 (h_a) 3.98 (h_c) 3.49	27.67 26.18 15.96 15.14 13.84 3.52	10 01 11 -21 20 45	a = 30.50 b = 28.86 γ = 65.15°
	Col_{ob} (28)	27.31 25.68 15.02 13.38 4.60 (h_a) 4.0 (h_c) 3.47	27.31 25.68 15.02 13.66 3.35	10 01 11 20 54	a = 32.81 b = 30.85 γ = 56.4° S = 842.68 V = 3365.3
PBI-Se[10] (44.6) MW: 1461.13	Col_h (200)	28.30 16.30 14.08 5.90 4.82 (h_a)	28.30 16.34 14.15	10 11 20	a = 32.68
	Col_h (100)	28.00 16.14 13.93 4.65 (h_a) 3.73 (h_c)	28.01 16.17 14.00	10 11 20	a = 32.34
	Col_h (28)	27.58 15.89 13.71	27.58 15.93 13.79	10 11 20	a = 31.85 S = 878.5 V = 3660.2

		4.56 4.176 (h_a) 3.74 (h_c)	3.83	62	

[a]The diameter (D) of the disk (estimated from Chem 3D Pro 8.0 molecular model software from Cambridge Soft). d_{obs}: spacing observed; d_{cal}: spacing calculated (deduced from the lattice parameters; a for Col_h phase; a, b for Col_{ob} phase; γ is the tilt angle for Col_{ob} phase; c is height of the unit cell). The spacings marked h_a and h_c correspond to diffuse reflections in the wide-angle region arising from correlations between the alkyl chains and core regions, respectively.

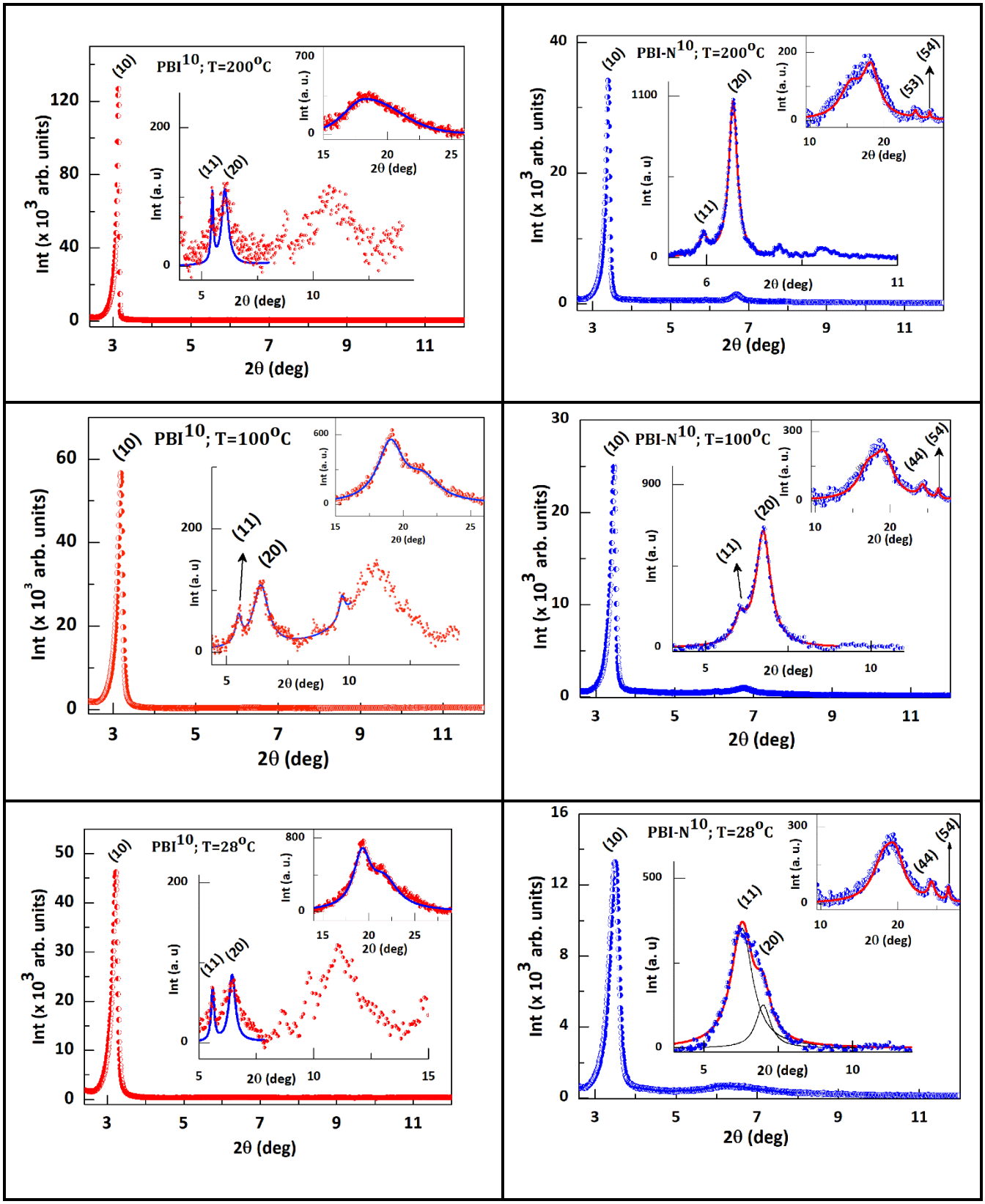


Figure S26. XRD pattern obtained for compound **PBI**^{10} (left) and **PBI-N**^{10} (right) at different temperature intervals.

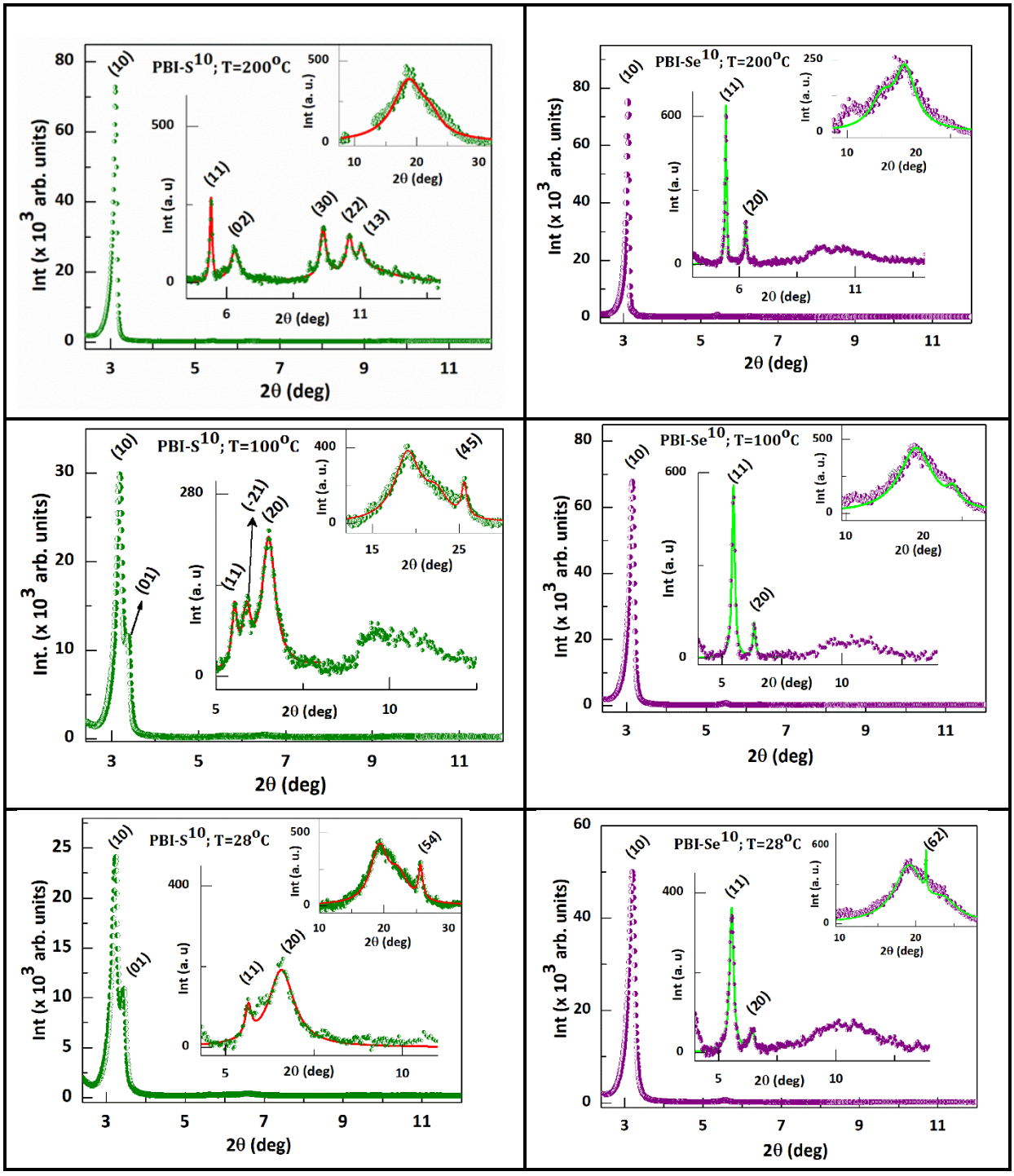


Figure S27. XRD pattern obtained for compound **PBI-S**[10] (left) and **PBI-Se**[10] (right) at different temperature intervals.

10. Device Fabrication and Characterizations

Based on superior photophysical and electrochemical properties, the electroluminescent properties of **PBI-N**[10]**, PBI**[10]**, PBI-S**[10], and **PBI-Se**[10] emitter materials. Multi-layered solution processed OLEDs were fabricated consisting of following device configurations: indium tin-oxide (ITO)/ PEDOT:PSS (35 nm)/ PVK (20 nm)/ **PBI-N**[10] or **PBI**[10] or **PBI-S**[10], or **PBI-Se**[10]

(20 nm)/ TPBi (40 nm)/ LiF (0.5 nm)/ Al (200 nm) for non-doped device and ITO/ PEDOT:PSS (35 nm)/ PVK (20 nm)/ CBP: **PBI-N**[10] or **PBI**[10] or **PBI-S**[10], or **PBI-Se**[10] (1,3 and 5 wt%) (20 nm)/ TPBi (40 nm)/ LiF (0.5 nm)/ Al (200 nm) for doped device. Initially, ITO-coated glass substrates were cleaned to remove greasy layer. The cleaning process was carried-out with soap-solution, deionized water, acetone, and alcohol in water-bath sonicator at optimized time. Cleaned substrates were kept in ultra-violet ozone system to expose in UV-light for removing residual solvents and further impurities. Then, these substrates were transferred into nitrogen purged glovebox for further processing of layers. Simultaneously, the PVK for HTM and CBP as host and newly synthesized emitters for emissive solution layer were dispersed into suitable solvents with water-bath sonicator. Prepared solutions were filtered with 0.45 µm PTFE filters and mixed in desired ratio to prepare emissive layer. First, a hole-injection layer was prepared by spin-coating an aqueous solution of PEDOT:PSS at 4,000 rpm for 20 s. Subsequently, these substrates were annealed at 130 ^{o}C for 15 minutes. Then, a solution of HTM was spin-coated onto hole-injection layer to form a thin-layer of hole transport layer. After that, these samples were treated by 70 ^{o}C for 30 minutes to remove the solvent. After cooled down the substrates, neat solution or emissive layer solution were spin-coated onto hole-transport layer at 2,500 rpm for 20 s. Then, these substrates were transferred into thermal evaporator to deposit subsequent layers. Then, TPBi was deposited as an electron-transport layer followed by the deposition of 0.5 nm LiF as an electron-injection layer and 200 nm Al as a cathode. All the layers of TPBi, LiF and Al were deposited subsequentially via thermal evaporation method at base pressure of 4.0×10^{-6} Torr. After that, Fabricated devices were kept in the mini vacuum chamber during testing process and then measured at room temperature conditions. To analyse the device, the electroluminescence (EL) spectrum, luminance, and the CIE coordinates were obtained using a photo research (PR-655) spectrometer. The current density-voltage-luminance (J-V-L) characteristics were obtained by a computer mounted voltmeter (Keithley 2400) and spectrophotometer CS-100 Minolta. Lifetime measurement was carried-out with computer mounted Lifetime Test System. Lifetime was investigated without encapsulation of devices.

Table S4. Effect of doping concentration on the operation voltage (Von), power efficacy (PE), current efficacy (CE), external quantum efficacy (EQE), CIE coordinates, and maximum luminance of solution-processed deep-red/NIR OLED devices with the CBP host for **PBI-N**[10], **PBI**[10], **PBI-S**[10], and **PBI-Se**[10].

Hosts	Dopant Concen. (wt%)	V_{on} (V)	Power efficacy (lm/W)			Current efficacy (cd/A)			External quantum efficiency (%)			CIE_{xy} @100 cd/m^2	L_{max} cd/m^2
			Max.	100 cd/m^2	1,000 cd/m^2	Max.	100 cd/m^2	1,000 cd/m^2	Max.	100 cd/m^2	1,000 cd/m^2		
PBI-N[10]	1.0	3.0	7.2	4.0	2.4	6.9	5.3	4.2	4.9	4.4	3.2	(0.46,0.32)	2,900
	3.0	3.2	2.1	1.3	0.8	2.3	2.0	1.6	2.9	2.9	1.7	(0.54,0.30)	1,820
	5.0	3.5	0.6	0.4	0.5	1.1	0.8	1.0	1.9	1.3	1.2	(0.52,0.27)	1294
	100	3.6	0.6	0.3	-	0.7	0.5	-	0.9	0.9	-	(0.52,0.27)	676
PBI[10]	1.0	3.0	2.4	1.8	0.8	2.7	2.7	1.6	4.3	4.3	1.8	(0.44,0.28)	1,366
	3.0	3.6	0.9	0.8	-	1.3	1.3	-	2.9	2.9	-	(0.39,0.20)	886
	5.0	3.7	0.5	0.4	-	0.6	0.6	-	2.0	1.8	-	(0.33,0.16)	612
	100	4.0	0.2	0.1	-	0.4	0.3	-	0.9	0.8	-	(0.33,0.15)	294
PBI-S[10]	1.0	3.3	1.3	0.8	-	1.3	1.3	-	2.1	2.0	-	(0.43,0.25)	683
	3.0	3.8	0.5	0.3	-	0.6	0.6	-	1.4	1.4	-	(0.39,0.20)	443
	5.0	4.0	0.2	0.2	-	0.3	0.3	-	0.9	0.9	-	(0.33,0.16)	306
	100	4.1	0.2	0.1	-	0.3	0.3	-	0.8	0.8	-	(0.33,0.16)	293
PBI-Se[10]	1.0	4.0	1.2	1.2	-	1.4	1.3	-	1.6	1.6	-	(0.40,0.23)	210
	3.0	4.1	0.7	0.7	-	1.1	1.1	-	1.6	1.6	-	(0.40,0.23)	191
	5.0	4.2	0.6	0.4	-	0.8	0.8	-	1.5	1.5	-	(0.40,0.23)	140
	100	4.0	0.3	0.2	-	0.3	0.3	-	0.9	0.9	-	(0.33,0.16)	177

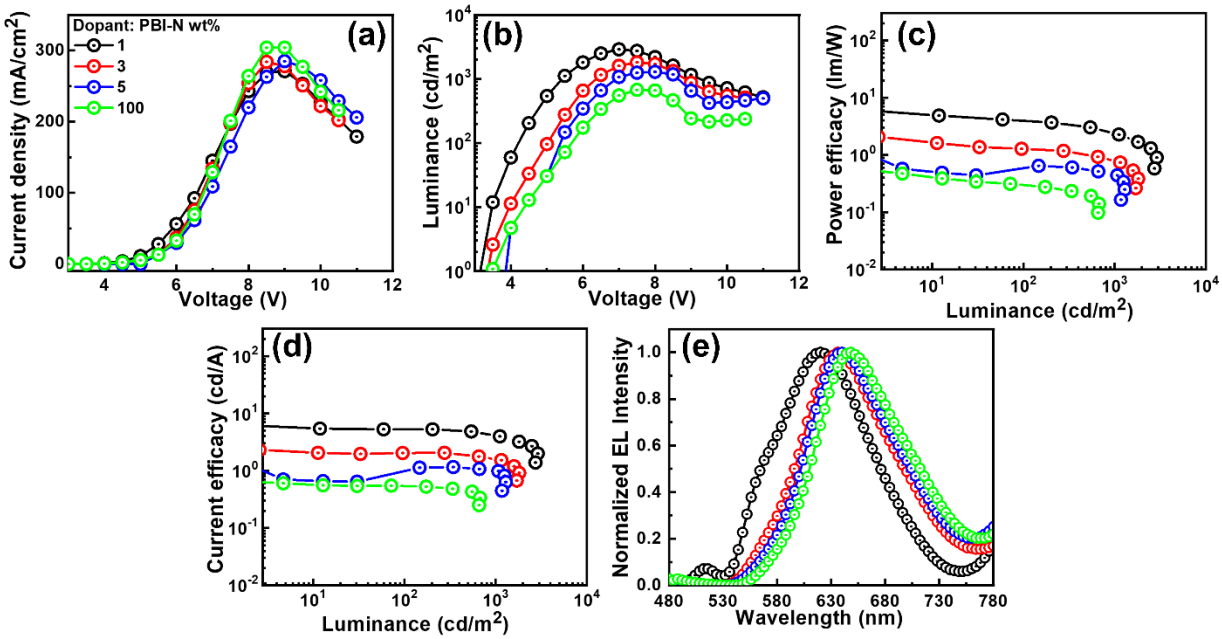


Figure S28. (a) Current density-voltage, (b) luminance-voltage, (c) power efficacy-luminance, (d) current efficacy-luminance, and (e) EL spectra curves of the solution-processed deep-red/NIR OLED using CBP host with 1, 3, 5, and 100 wt% **PBI-N**[10] concentration.

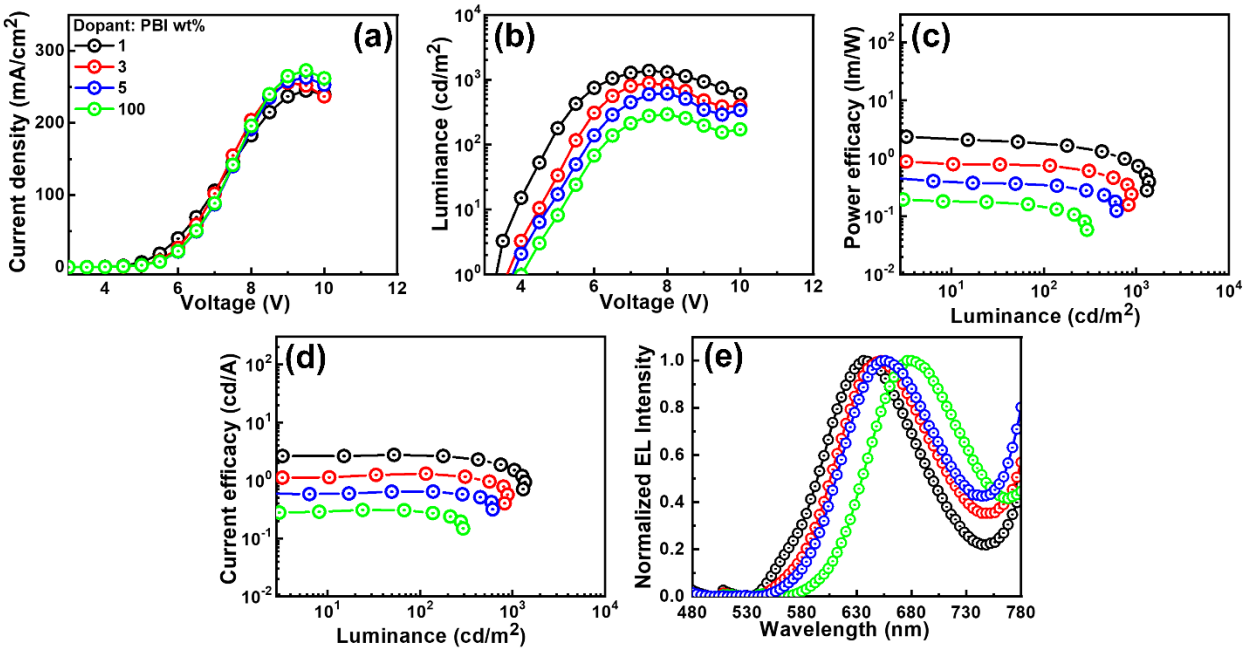


Figure S29. (a) Current density-voltage, (b) luminance-voltage, (c) power efficacy-luminance, (d) current efficacy-luminance, and (e) EL spectra curves of the solution-processed deep-red/NIR OLED using CBP host with 1, 3, 5, and 100 wt% **PBI**[10] concentration.

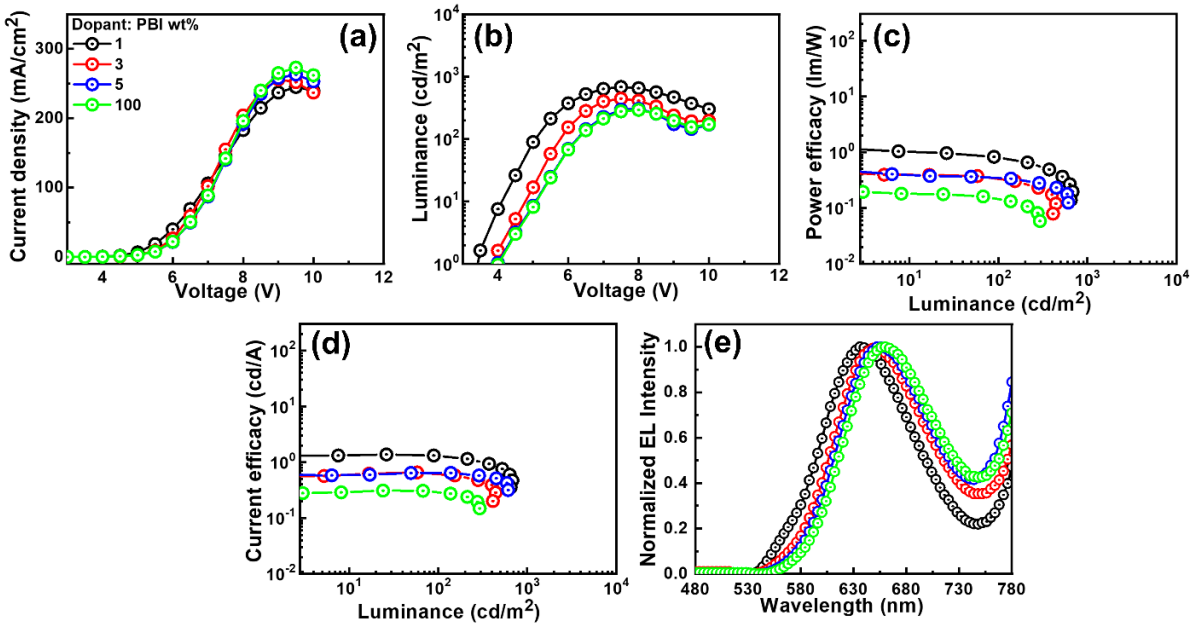


Figure S30. (a) Current density-voltage, (b) luminance-voltage, (c) power efficacy-luminance, (d) current efficacy-luminance, and (e) EL spectra curves of the solution-processed deep-red/NIR OLED using CBP host with 1, 3, 5, and 100 wt% **PBI-S**[10] concentration.

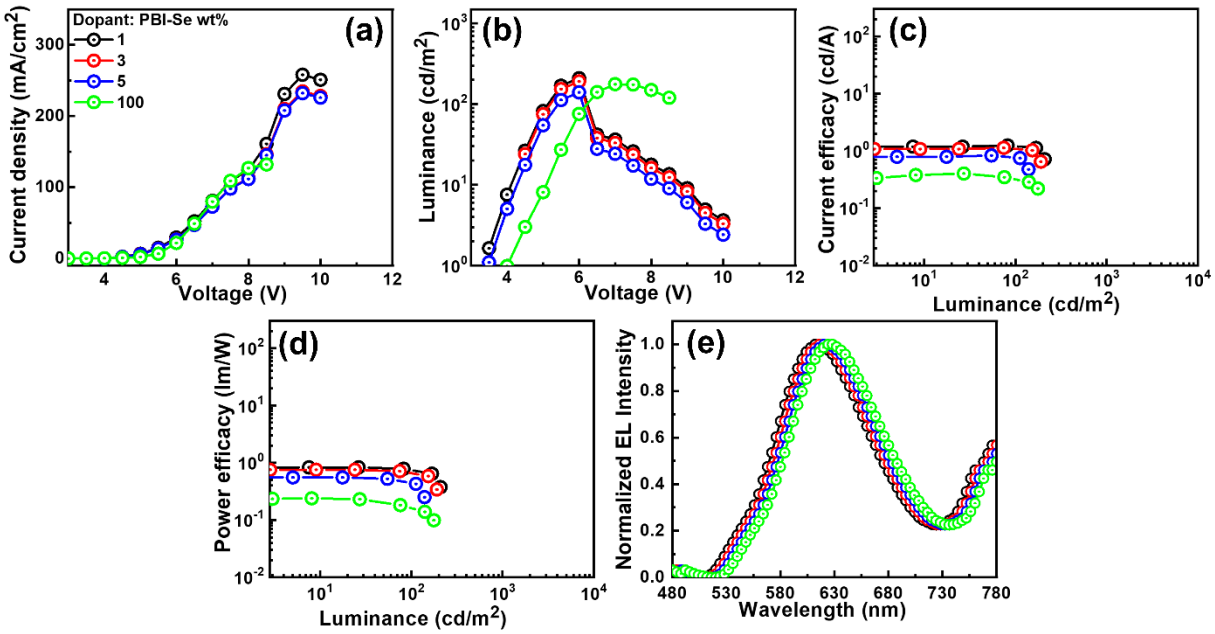


Figure S31. (a) Current density-voltage, (b) luminance-voltage, (c) power efficacy-luminance, (d) current efficacy-luminance, and (e) EL spectra curves of the solution-processed deep-red/NIR OLED using CBP host with 1, 3, 5, and 100 wt% **PBI-Se**[10] concentration.

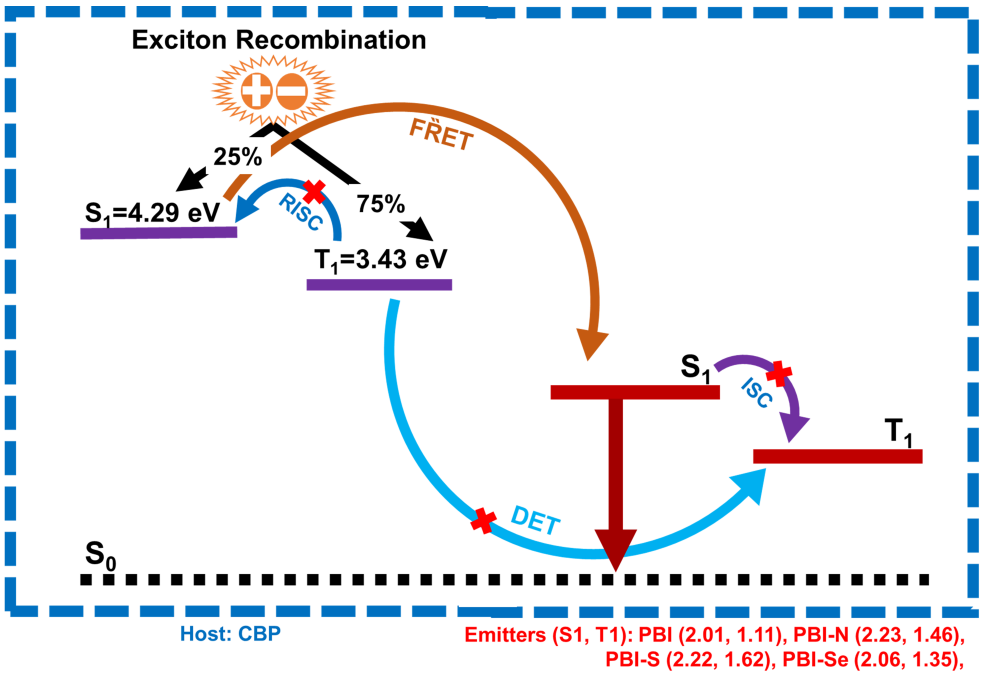


Figure S32. Energy-transfer routes from host-to-guest.

11. DFT Studies

To understand the electronic properties and frontier molecular orbital energy level of compounds **PBI**[10], **PBI-N**[10], **PBI-S**[10] and **PBI-Se**[10], computational studies was carried out in B3LYP/6-31g (dp) method using Gaussian 09 program package.[S4] The absence of imaginary frequency ensured the energy minimized structure of all the compounds.

DFT calculation data for **PBI**[10]**:**

Center No.	Atomic No.	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.589292	2.134638	1.696953
2	6	0	-1.199175	2.050152	1.565907
3	6	0	-0.588688	1.054871	0.800161
4	6	0	-1.419109	0.097550	0.135523
5	6	0	-2.838853	0.191309	0.275746
6	6	0	-3.411342	1.220073	1.061828
7	6	0	-0.865884	-0.951253	-0.665809
8	6	0	-1.738038	-1.849569	-1.283720
9	6	0	-3.125912	-1.750672	-1.140266
10	6	0	-3.682221	-0.744032	-0.370326
11	6	0	0.871477	0.958858	0.655382
12	6	0	1.424704	-0.090027	-0.145844
13	6	0	0.594279	-1.047348	-0.810476
14	6	0	1.743656	1.857158	1.273287
15	6	0	3.131541	1.758127	1.129981
16	6	0	3.687857	0.751281	0.360312
17	6	0	2.844461	-0.184035	-0.285760
18	6	0	3.416944	-1.213181	-1.071344
19	6	0	2.594887	-2.127697	-1.706526

20	6	0	1.204753	-2.042853	-1.575936
21	6	0	-5.158761	-0.667870	-0.240822
22	7	0	-5.671004	0.381303	0.551090
23	6	0	-4.882359	1.340439	1.220021
24	6	0	5.164426	0.674734	0.231274
25	7	0	5.676671	-0.375094	-0.559780
26	6	0	4.887986	-1.334165	-1.228750
27	8	0	-5.394217	2.222016	1.891775
28	8	0	-5.901158	-1.467778	-0.787982
29	8	0	5.906859	1.474396	0.778745
30	8	0	5.399848	-2.216321	-1.899740
31	6	0	-7.109085	0.481701	0.682817
32	6	0	7.114796	-0.476815	-0.690009
33	6	0	-7.790361	1.532311	0.080931
34	6	0	-9.177291	1.645989	0.205361
35	6	0	-9.902246	0.670697	0.932328
36	6	0	-9.203135	-0.409161	1.520544
37	6	0	-7.809689	-0.475470	1.401833
38	6	0	7.794451	-1.527289	-0.086086
39	6	0	9.181382	-1.642519	-0.208928
40	6	0	9.908029	-0.668980	-0.936561
41	6	0	9.210564	0.410827	-1.526844
42	6	0	7.817067	0.478770	-1.409515
43	6	0	-12.987749	-12.633309	1.022455
44	6	0	-12.910464	-11.359000	1.868758
45	6	0	-12.222735	-10.193419	1.147502
46	6	0	-12.143612	-8.911090	1.984887
47	6	0	-11.456671	-7.747387	1.259897
48	6	0	-11.380132	-6.461263	2.092000
49	6	0	-10.697970	-5.299781	1.358861
50	6	0	-10.624175	-4.007908	2.182474
51	6	0	-9.952266	-2.850990	1.433787
52	6	0	-9.876173	-1.551784	2.262814
53	6	0	-21.317810	-2.319049	-4.076554
54	6	0	-20.568556	-1.570327	-2.970251
55	6	0	-19.044445	-1.707858	-3.070494
56	6	0	-18.284814	-0.963983	-1.965391
57	6	0	-16.761099	-1.103555	-2.068488
58	6	0	-15.998135	-0.364297	-0.962337
59	6	0	-14.475138	-0.509358	-1.069321
60	6	0	-13.706147	0.221488	0.038374
61	6	0	-12.184829	0.067478	-0.076323
62	6	0	-11.413495	0.788297	1.048307
63	6	0	-12.575183	13.925582	1.566069
64	6	0	-12.556292	12.698571	0.649555
65	6	0	-11.914346	11.466477	1.298970
66	6	0	-11.890224	10.232917	0.388260
67	6	0	-11.247731	9.001525	1.038463
68	6	0	-11.219164	7.769409	0.125651
69	6	0	-10.577292	6.537896	0.776396
70	6	0	-10.539651	5.309401	-0.141063
71	6	0	-9.897850	4.079129	0.511067
72	6	0	-9.837249	2.857950	-0.429142
73	6	0	12.501483	-13.949899	-1.509546
74	6	0	12.492770	-12.717238	-0.600493
75	6	0	11.864003	-11.482928	-1.258540

76	6	0	11.849431	-10.243981	-0.354969
77	6	0	11.218737	-9.010697	-1.013092
78	6	0	11.198070	-7.773817	-0.106533
79	6	0	10.565526	-6.541001	-0.763914
80	6	0	10.533337	-5.308684	0.148614
81	6	0	9.897524	-4.077912	-0.508424
82	6	0	9.839320	-2.854064	0.428462
83	6	0	21.320714	2.318150	4.080419
84	6	0	20.572004	1.568204	2.974578
85	6	0	19.047919	1.707529	3.072726
86	6	0	18.288836	0.962452	1.968056
87	6	0	16.765145	1.103784	2.069081
88	6	0	16.002737	0.363357	0.963328
89	6	0	14.479760	0.510108	1.068286
90	6	0	13.711337	-0.221846	-0.039073
91	6	0	12.190035	-0.066239	0.073659
92	6	0	11.419298	-0.788092	-1.050719
93	6	0	13.010927	12.630406	-1.037811
94	6	0	12.932927	11.355291	-1.882832
95	6	0	12.242440	10.191530	-1.161275
96	6	0	12.162575	8.908403	-1.997365
97	6	0	11.472956	7.746501	-1.272029
98	6	0	11.395676	6.459567	-2.102811
99	6	0	10.711003	5.299841	-1.369234
100	6	0	10.636479	4.007141	-2.191482
101	6	0	9.962301	2.851915	-1.442224
102	6	0	9.885518	1.551849	-2.269835
103	1	0	-3.046644	2.914859	2.295211
104	1	0	-0.596825	2.788086	2.081159
105	1	0	-1.349019	-2.653812	-1.895893
106	1	0	-3.788684	-2.457401	-1.627188
107	1	0	1.354653	2.661451	1.885404
108	1	0	3.794324	2.464806	1.616961
109	1	0	3.052249	-2.908206	-2.304401
110	1	0	0.602390	-2.780814	-2.091133
111	1	0	-7.236084	2.278099	-0.480449
112	1	0	-7.269678	-1.295305	1.865416
113	1	0	7.238888	-2.271734	0.475801
114	1	0	7.278345	1.298564	-1.874666
115	1	0	-13.481142	-13.446358	1.564949
116	1	0	-13.550437	-12.461218	0.097856
117	1	0	-11.988054	-12.981700	0.738808
118	1	0	-12.374588	-11.572563	2.803653
119	1	0	-13.923599	-11.053917	2.164142
120	1	0	-12.757444	-9.982180	0.210272
121	1	0	-11.208131	-10.498348	0.853279
122	1	0	-11.608584	-9.122201	2.921841
123	1	0	-13.158485	-8.607086	2.278856
124	1	0	-11.990484	-7.539399	0.321598
125	1	0	-10.441172	-8.050786	0.967858
126	1	0	-10.842831	-6.666251	3.028970
127	1	0	-12.395403	-6.158790	2.386161
128	1	0	-11.234142	-5.099227	0.420397
129	1	0	-9.682139	-5.601097	1.066580
130	1	0	-10.080161	-4.202823	3.117866
131	1	0	-11.639545	-3.709131	2.480531

132	1	0	-10.493796	-2.653878	0.499735
133	1	0	-8.938368	-3.144664	1.132883
134	1	0	-9.308640	-1.758452	3.179697
135	1	0	-10.883744	-1.278750	2.588341
136	1	0	-22.401754	-2.198777	-3.979725
137	1	0	-21.030026	-1.951978	-5.068333
138	1	0	-21.098737	-3.392502	-4.047112
139	1	0	-20.900978	-1.937683	-1.989775
140	1	0	-20.838366	-0.505871	-3.001277
141	1	0	-18.711680	-1.339271	-4.051497
142	1	0	-18.775206	-2.773548	-3.042034
143	1	0	-18.617750	-1.333382	-0.984853
144	1	0	-18.554497	0.101476	-1.993793
145	1	0	-16.428270	-0.732446	-3.048338
146	1	0	-16.492540	-2.169337	-2.042933
147	1	0	-16.330462	-0.735254	0.017781
148	1	0	-16.264375	0.702064	-0.987597
149	1	0	-14.142790	-0.135513	-2.048188
150	1	0	-14.210917	-1.576247	-1.048913
151	1	0	-14.037397	-0.152285	1.017889
152	1	0	-13.967094	1.289438	0.019110
153	1	0	-11.848140	0.449573	-1.049114
154	1	0	-11.923810	-0.998028	-0.068382
155	1	0	-11.749974	0.395852	2.013118
156	1	0	-11.702898	1.843758	1.051755
157	1	0	-13.037491	14.787342	1.073678
158	1	0	-13.139041	13.725723	2.484342
159	1	0	-11.560194	14.216092	1.860258
160	1	0	-12.016903	12.941579	-0.276090
161	1	0	-13.583039	12.453392	0.345368
162	1	0	-12.453996	11.223739	2.225663
163	1	0	-10.887126	11.712661	1.604178
164	1	0	-11.350593	10.476920	-0.538016
165	1	0	-12.917576	9.987584	0.083079
166	1	0	-11.789079	8.755539	1.963118
167	1	0	-10.221503	9.247789	1.346300
168	1	0	-10.676397	8.015580	-0.798185
169	1	0	-12.245086	7.523369	-0.183721
170	1	0	-11.123646	6.287263	1.696750
171	1	0	-9.553664	6.785263	1.091206
172	1	0	-9.990958	5.560401	-1.060185
173	1	0	-11.562794	5.061857	-0.458904
174	1	0	-10.451322	3.813282	1.421590
175	1	0	-8.879213	4.321674	0.840362
176	1	0	-9.267758	3.136634	-1.324324
177	1	0	-10.846384	2.619469	-0.780316
178	1	0	12.954397	-14.813125	-1.011030
179	1	0	11.484283	-14.232280	-1.804015
180	1	0	13.069056	-13.761123	-2.427875
181	1	0	13.521260	-12.480182	-0.295749
182	1	0	11.949267	-12.949407	0.325525
183	1	0	10.835178	-11.721195	-1.564628
184	1	0	12.407966	-11.250682	-2.185399
185	1	0	12.878415	-10.005993	-0.049466
186	1	0	11.306174	-10.477934	0.571777
187	1	0	10.191214	-9.250116	-1.322007

188	1	0	11.764184	-8.773929	-1.937742
189	1	0	12.225350	-7.533575	0.202897
190	1	0	10.652472	-8.011554	0.817841
191	1	0	9.541048	-6.783307	-1.079891
192	1	0	11.115401	-6.297560	-1.684100
193	1	0	11.557419	-5.064790	0.466256
194	1	0	9.982833	-5.553549	1.068304
195	1	0	8.878617	-4.317711	-0.838889
196	1	0	10.453638	-3.816650	-1.418663
197	1	0	10.848826	-2.616599	0.779265
198	1	0	9.269155	-3.129422	1.324241
199	1	0	22.404646	2.196551	3.985124
200	1	0	21.102819	3.391779	4.048752
201	1	0	21.031339	1.953198	5.072517
202	1	0	20.840646	0.503521	3.007870
203	1	0	20.905999	1.933419	1.993836
204	1	0	18.779845	2.773450	3.042006
205	1	0	18.713580	1.341077	4.053993
206	1	0	18.557379	-0.103233	1.998697
207	1	0	18.623324	1.329740	0.987253
208	1	0	16.497720	2.169796	2.041320
209	1	0	16.430761	0.734753	3.049188
210	1	0	16.267888	-0.703221	0.990752
211	1	0	16.336571	0.732281	-0.017045
212	1	0	14.216620	1.577222	1.045770
213	1	0	14.145902	0.138244	2.047394
214	1	0	13.971268	-1.290005	-0.017759
215	1	0	14.044038	0.150008	-1.018826
216	1	0	11.930015	0.999496	0.063759
217	1	0	11.851894	-0.446498	1.046666
218	1	0	11.707782	-1.843805	-1.052273
219	1	0	11.757165	-0.397379	-2.015747
220	1	0	13.506300	13.442124	-1.580494
221	1	0	12.011357	12.980601	-0.755952
222	1	0	13.572056	12.458484	-0.112233
223	1	0	13.946020	11.048373	-2.176454
224	1	0	12.398690	11.568634	-2.818715
225	1	0	11.227880	10.498295	-0.868811
226	1	0	12.775516	9.980518	-0.223063
227	1	0	13.177401	8.602594	-2.289620
228	1	0	11.629129	9.119267	-2.935277
229	1	0	10.457506	8.051694	-0.981698
230	1	0	12.005198	7.538775	-0.332780
231	1	0	12.410897	6.155366	-2.395360
232	1	0	10.859835	6.664258	-3.040681
233	1	0	9.695221	5.602867	-1.078556
234	1	0	11.245732	5.099611	-0.429877
235	1	0	11.651802	3.706747	-2.488076
236	1	0	10.093747	4.201688	-3.127695
237	1	0	8.948439	3.147185	-1.142762
238	1	0	10.502567	2.655199	-0.507355
239	1	0	10.893088	1.277329	-2.594112
240	1	0	9.319057	1.758081	-3.187481

DFT calculation data for **PBI-N^{10}:**

Center No.	Atomic No.	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.066270	2.278547	-1.942425
2	6	0	-1.706103	2.459640	-2.199926
3	6	0	-0.772835	1.466277	-1.901699
4	6	0	-1.346466	0.300816	-1.336611
5	6	0	-2.697034	0.087491	-1.061504
6	6	0	-3.579205	1.118482	-1.376290
7	6	0	-0.521866	-0.750977	-1.015099
8	6	0	-0.850718	-1.984034	-0.467409
9	6	0	-2.217389	-2.165318	-0.191938
10	6	0	-3.112715	-1.139288	-0.484512
11	6	0	0.672910	1.516819	-2.108909
12	6	0	1.455451	0.399895	-1.729666
13	6	0	0.827756	-0.705641	-1.208399
14	6	0	1.420179	2.558262	-2.660929
15	6	0	2.807953	2.469232	-2.797120
16	6	0	3.533071	1.359286	-2.384037
17	6	0	2.838433	0.283462	-1.836177
18	6	0	3.479292	-0.921798	-1.453058
19	6	0	2.775544	-2.012138	-0.949877
20	6	0	1.379477	-1.913256	-0.800653
21	6	0	-4.518946	-1.306980	-0.178600
22	7	0	-5.400302	-0.253017	-0.502088
23	6	0	-4.992802	0.948741	-1.121012
24	6	0	4.975128	1.276640	-2.499254
25	7	0	5.609381	0.250340	-1.750593
26	6	0	4.920727	-0.985381	-1.603567
27	8	0	-5.823750	1.790665	-1.443563
28	8	0	-4.947192	-2.311707	0.382487
29	8	0	5.620994	2.064813	-3.176366
30	8	0	5.526838	-2.049198	-1.573569
31	6	0	-6.774760	-0.405498	-0.170620
32	6	0	6.907223	0.438179	-1.206632
33	6	0	-7.457269	0.573952	0.527320
34	6	0	-8.794154	0.454429	0.871319
35	6	0	-9.490364	-0.712857	0.536854
36	6	0	-8.820944	-1.706652	-0.185888
37	6	0	-7.489861	-1.534695	-0.526265
38	6	0	7.527607	-0.507242	-0.397658
39	6	0	8.782842	-0.344171	0.168846
40	6	0	9.475765	0.859178	-0.003416
41	6	0	8.855634	1.855708	-0.764054
42	6	0	7.603835	1.636440	-1.318360
43	7	0	0.330092	-2.680215	-0.350383
44	6	0	0.453407	-4.044904	0.182967
45	6	0	0.685108	-4.051685	1.695625
46	6	0	-11.583203	-13.714968	3.121357
47	6	0	-11.746670	-12.623896	2.057743
48	6	0	-11.001714	-11.332270	2.421343
49	6	0	-11.162251	-10.232600	1.361823
50	6	0	-10.420111	-8.939672	1.729963
51	6	0	-10.584477	-7.835205	0.675834
52	6	0	-9.850652	-6.540378	1.054001
53	6	0	-10.022790	-5.427631	0.010153

54	6	0	-9.303538	-4.129777	0.407151
55	6	0	-9.482086	-3.005205	-0.626822
56	6	0	-21.833305	1.941672	-1.525036
57	6	0	-20.811518	1.210103	-0.648013
58	6	0	-19.373130	1.377071	-1.156686
59	6	0	-18.343878	0.648511	-0.280719
60	6	0	-16.903609	0.818650	-0.785454
61	6	0	-15.875980	0.095963	0.097479
62	6	0	-14.432723	0.274237	-0.395656
63	6	0	-13.408562	-0.434383	0.502389
64	6	0	-11.960809	-0.238411	0.027873
65	6	0	-10.941045	-0.911175	0.959666
66	6	0	-13.072254	12.425534	-0.240484
67	6	0	-12.928388	11.210395	0.682103
68	6	0	-12.187034	10.046691	0.009979
69	6	0	-12.039683	8.824209	0.927340
70	6	0	-11.297984	7.660879	0.253134
71	6	0	-11.152361	6.435560	1.167090
72	6	0	-10.412395	5.273800	0.488293
73	6	0	-10.271518	4.043185	1.395490
74	6	0	-9.541112	2.882474	0.703432
75	6	0	-9.405922	1.641162	1.606188
76	6	0	13.387411	-12.242559	-0.338867
77	6	0	13.080991	-11.036390	0.555363
78	6	0	12.454605	-9.871415	-0.223094
79	6	0	12.144300	-8.658587	0.665962
80	6	0	11.516010	-7.494593	-0.114036
81	6	0	11.204142	-6.280825	0.773415
82	6	0	10.573226	-5.119888	-0.008994
83	6	0	10.259674	-3.904550	0.875200
84	6	0	9.630405	-2.747316	0.084817
85	6	0	9.311968	-1.527533	0.969985
86	6	0	22.086799	-1.260190	-0.201849
87	6	0	20.911555	-0.606037	0.532480
88	6	0	19.577760	-0.800160	-0.201514
89	6	0	18.395456	-0.149249	0.530568
90	6	0	17.059311	-0.346578	-0.200077
91	6	0	15.877798	0.298388	0.538695
92	6	0	14.537435	0.092808	-0.181925
93	6	0	13.357561	0.723958	0.571148
94	6	0	12.010587	0.501029	-0.132722
95	6	0	10.830804	1.098162	0.650356
96	6	0	10.477177	13.636363	3.868925
97	6	0	10.841055	12.651204	2.752922
98	6	0	10.119969	11.304376	2.899741
99	6	0	10.481163	10.310039	1.786817
100	6	0	9.762908	8.961333	1.938628
101	6	0	10.128738	7.961757	0.831761
102	6	0	9.418820	6.609974	0.994732
103	6	0	9.793561	5.601112	-0.100490
104	6	0	9.098536	4.243858	0.083115
105	6	0	9.482406	3.222837	-1.001082
106	1	0	-3.733346	3.089212	-2.198151
107	1	0	-1.402848	3.400116	-2.638021
108	1	0	-2.556685	-3.091908	0.249008
109	1	0	0.945609	3.468926	-2.998699

110	1	0	3.324968	3.316021	-3.225559
111	1	0	3.289432	-2.915985	-0.654437
112	1	0	-6.927901	1.461526	0.845150
113	1	0	-7.003604	-2.310440	-1.101214
114	1	0	7.035726	-1.427500	-0.135315
115	1	0	7.178651	2.486490	-1.823348
116	1	0	-0.446601	-4.615196	-0.058253
117	1	0	1.273004	-4.561923	-0.321575
118	1	0	0.774056	-5.074418	2.072424
119	1	0	1.603242	-3.517857	1.955892
120	1	0	-0.143396	-3.571342	2.223221
121	1	0	-12.121995	-14.626203	2.842444
122	1	0	-10.529919	-13.981441	3.255544
123	1	0	-11.972059	-13.384303	4.089776
124	1	0	-12.813561	-12.404063	1.929962
125	1	0	-11.374430	-12.999804	1.097029
126	1	0	-9.935419	-11.556836	2.549142
127	1	0	-11.375392	-10.962134	3.384248
128	1	0	-12.228935	-10.010548	1.233150
129	1	0	-10.786305	-10.601883	0.399529
130	1	0	-9.352886	-9.160726	1.856008
131	1	0	-10.794063	-8.573820	2.694361
132	1	0	-11.652180	-7.618241	0.546352
133	1	0	-10.204459	-8.196694	-0.287800
134	1	0	-8.781998	-6.754916	1.178097
135	1	0	-10.226897	-6.185367	2.021495
136	1	0	-11.092585	-5.219685	-0.119760
137	1	0	-9.635947	-5.774907	-0.956239
138	1	0	-8.233477	-4.331075	0.533264
139	1	0	-9.681344	-3.797360	1.380799
140	1	0	-10.540658	-2.856457	-0.854043
141	1	0	-9.046281	-3.331132	-1.578741
142	1	0	-22.851141	1.809376	-1.144264
143	1	0	-21.629225	3.016721	-1.556483
144	1	0	-21.813196	1.565500	-2.552854
145	1	0	-21.063972	0.143292	-0.615980
146	1	0	-20.880521	1.591769	0.377896
147	1	0	-19.126130	2.445569	-1.189590
148	1	0	-19.308371	0.994562	-2.182919
149	1	0	-18.590241	-0.420146	-0.249317
150	1	0	-18.412201	1.029812	0.745776
151	1	0	-16.659053	1.887596	-0.819997
152	1	0	-16.832616	0.433071	-1.810069
153	1	0	-16.116386	-0.974032	0.128120
154	1	0	-15.954014	0.477711	1.123173
155	1	0	-14.196289	1.344882	-0.433767
156	1	0	-14.348468	-0.116828	-1.417143
157	1	0	-13.636953	-1.507238	0.534206
158	1	0	-13.504145	-0.049009	1.525520
159	1	0	-11.753731	0.834009	-0.033471
160	1	0	-11.850176	-0.644803	-0.984241
161	1	0	-11.185781	-1.972857	1.038222
162	1	0	-11.083394	-0.566623	1.988493
163	1	0	-13.603132	13.242874	0.258099
164	1	0	-12.093140	12.806195	-0.548246
165	1	0	-13.633044	12.170459	-1.145375

166	1	0	-13.925443	10.874928	0.992409
167	1	0	-12.388640	11.509547	1.588771
168	1	0	-11.191033	10.387031	-0.299688
169	1	0	-12.728849	9.752857	-0.897648
170	1	0	-13.036047	8.484534	1.236517
171	1	0	-11.497988	9.118511	1.834891
172	1	0	-10.301182	8.000386	-0.054746
173	1	0	-11.838773	7.368911	-0.655680
174	1	0	-12.149328	6.096235	1.474948
175	1	0	-10.610062	6.726023	2.075552
176	1	0	-9.414570	5.611997	0.182987
177	1	0	-10.952908	4.987595	-0.422473
178	1	0	-11.270794	3.709288	1.703209
179	1	0	-9.724431	4.323644	2.304584
180	1	0	-8.550329	3.224500	0.385905
181	1	0	-10.086574	2.609387	-0.206564
182	1	0	-10.386469	1.415587	2.025346
183	1	0	-8.773579	1.890035	2.467821
184	1	0	13.832802	-13.060881	0.235992
185	1	0	12.476996	-12.626729	-0.809949
186	1	0	14.090602	-11.976251	-1.134407
187	1	0	14.008860	-10.697502	1.031900
188	1	0	12.398462	-11.346861	1.355831
189	1	0	11.528021	-10.215514	-0.699403
190	1	0	13.139577	-9.565545	-1.023659
191	1	0	13.071257	-8.314326	1.141245
192	1	0	11.460225	-8.965457	1.466989
193	1	0	10.589462	-7.839463	-0.589690
194	1	0	12.200053	-7.187839	-0.915002
195	1	0	12.130911	-5.933978	1.247299
196	1	0	10.520955	-6.587339	1.575346
197	1	0	9.647371	-5.467548	-0.483612
198	1	0	11.256418	-4.813664	-0.810857
199	1	0	11.186786	-3.557599	1.349343
200	1	0	9.574396	-4.207836	1.677015
201	1	0	8.717687	-3.106587	-0.402299
202	1	0	10.317018	-2.444410	-0.713684
203	1	0	10.208004	-1.280898	1.539240
204	1	0	8.564506	-1.812664	1.721671
205	1	0	23.026809	-1.109562	0.338623
206	1	0	21.935396	-2.339158	-0.307687
207	1	0	22.210463	-0.838284	-1.204377
208	1	0	21.110953	0.466446	0.646120
209	1	0	20.836605	-1.031532	1.540616
210	1	0	19.383982	-1.874070	-0.315151
211	1	0	19.656954	-0.373636	-1.209239
212	1	0	18.588980	0.924849	0.642694
213	1	0	18.319709	-0.574675	1.539059
214	1	0	16.867936	-1.420750	-0.314992
215	1	0	17.132019	0.082698	-1.207046
216	1	0	16.065733	1.373622	0.649364
217	1	0	15.811176	-0.127013	1.547885
218	1	0	14.354294	-0.982542	-0.299036
219	1	0	14.597155	0.526750	-1.187662
220	1	0	13.534366	1.801358	0.681465
221	1	0	13.308227	0.295485	1.580343

222	1	0	11.858071	-0.574084	-0.267267
223	1	0	12.042567	0.948973	-1.132868
224	1	0	11.017570	2.163721	0.799904
225	1	0	10.826686	0.720098	1.677324
226	1	0	11.001941	14.589105	3.745132
227	1	0	9.403271	13.848621	3.874098
228	1	0	10.745341	13.236472	4.852064
229	1	0	11.925158	12.485319	2.759802
230	1	0	10.585887	13.096078	1.783473
231	1	0	9.036178	11.474971	2.892996
232	1	0	10.375606	10.865265	3.872171
233	1	0	11.565399	10.142452	1.792881
234	1	0	10.223015	10.748034	0.814672
235	1	0	8.678525	9.127915	1.929007
236	1	0	10.018083	8.526931	2.913262
237	1	0	11.213899	7.800413	0.838033
238	1	0	9.867035	8.391133	-0.143244
239	1	0	8.333324	6.768991	0.981573
240	1	0	9.674973	6.187181	1.974252
241	1	0	10.880522	5.450642	-0.092661
242	1	0	9.526306	6.015047	-1.080770
243	1	0	8.011670	4.388271	0.069154
244	1	0	9.353088	3.845340	1.071850
245	1	0	10.568887	3.146398	-1.090689
246	1	0	9.164947	3.609411	-1.976383

DFT calculation data for **PBI-S[10]:**

Center No.	Atomic No.	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.146294	-2.743163	-0.305884
2	6	0	1.775020	-2.976693	-0.317620
3	6	0	0.849904	-1.924615	-0.299629
4	6	0	1.437191	-0.634804	-0.278634
5	6	0	2.816390	-0.365933	-0.262044
6	6	0	3.688682	-1.458144	-0.272057
7	6	0	0.600235	0.472852	-0.263494
8	6	0	1.001183	1.817680	-0.238295
9	6	0	2.391154	2.046505	-0.219808
10	6	0	3.278823	0.974239	-0.230480
11	6	0	-0.590541	-2.056371	-0.293065
12	6	0	-1.401777	-0.894360	-0.268292
13	6	0	-0.779484	0.346691	-0.258942
14	6	0	-1.309919	-3.258699	-0.299420
15	6	0	-2.700496	-3.277536	-0.269762
16	6	0	-3.467158	-2.112265	-0.238459
17	6	0	-2.806613	-0.880364	-0.241326
18	6	0	-3.503822	0.354093	-0.212757
19	6	0	-2.825830	1.569818	-0.211990
20	6	0	-1.417423	1.596646	-0.231612

21	6	0	4.703745	1.225591	-0.186658
22	7	0	5.567861	0.099297	-0.189881
23	6	0	5.117277	-1.245579	-0.256935
24	6	0	-4.909812	-2.162875	-0.181804
25	7	0	-5.596357	-0.921545	-0.138823
26	6	0	-4.950877	0.342991	-0.188560
27	8	0	5.923759	-2.169938	-0.322921
28	8	0	5.169358	2.360156	-0.106672
29	8	0	-5.531974	-3.220765	-0.128227
30	8	0	-5.616868	1.375089	-0.231415
31	6	0	6.963139	0.331912	-0.103138
32	6	0	-7.008919	-0.944501	-0.025995
33	6	0	7.739464	-0.308339	0.852767
34	6	0	9.106206	-0.094792	0.973177
35	6	0	9.739754	0.819113	0.118388
36	6	0	8.976633	1.457921	-0.869620
37	6	0	7.614681	1.206759	-0.961270
38	6	0	-7.660009	-0.211780	0.956804
39	6	0	-9.041033	-0.207794	1.098547
40	6	0	-9.824157	-0.993107	0.239914
41	6	0	-9.186179	-1.731489	-0.767450
42	6	0	-7.803134	-1.695550	-0.881396
43	16	0	-0.307721	2.796869	-0.225450
44	6	0	11.629027	13.718581	-3.271842
45	6	0	11.725087	12.274819	-3.780697
46	6	0	11.092892	11.266020	-2.809979
47	6	0	11.185007	9.816451	-3.312877
48	6	0	10.553393	8.807906	-2.339920
49	6	0	10.644937	7.357547	-2.840874
50	6	0	10.015142	6.351091	-1.864564
51	6	0	10.106164	4.899495	-2.361599
52	6	0	9.480383	3.897240	-1.378041
53	6	0	9.565887	2.442019	-1.872704
54	6	0	21.811243	-2.980259	-1.795334
55	6	0	20.883468	-1.905875	-1.214423
56	6	0	19.400263	-2.199498	-1.486282
57	6	0	18.465205	-1.128144	-0.903003
58	6	0	16.980066	-1.423234	-1.167921
59	6	0	16.047972	-0.355932	-0.572259
60	6	0	14.560454	-0.654913	-0.818704
61	6	0	13.634447	0.402776	-0.197108
62	6	0	12.143600	0.093240	-0.410604
63	6	0	11.226402	1.126898	0.265169
64	6	0	13.187750	-11.625448	4.668058
65	6	0	13.161009	-10.124601	4.983350
66	6	0	12.368808	-9.319260	3.942344
67	6	0	12.336676	-7.814057	4.251544
68	6	0	11.541537	-7.009599	3.210701
69	6	0	11.506456	-5.504391	3.520063
70	6	0	10.706821	-4.702570	2.480645
71	6	0	10.667687	-3.197630	2.789999
72	6	0	9.865675	-2.401160	1.747773
73	6	0	9.819361	-0.892146	2.060401
74	6	0	-10.813784	11.767215	5.184018
75	6	0	-11.076850	10.280944	5.456765
76	6	0	-10.486740	9.370364	4.369364

77	6	0	-10.743570	7.878619	4.636287
78	6	0	-10.147376	6.969092	3.549982
79	6	0	-10.395269	5.476021	3.818537
80	6	0	-9.786530	4.569928	2.736365
81	6	0	-10.018556	3.075087	3.007997
82	6	0	-9.392593	2.176609	1.928686
83	6	0	-9.601444	0.675190	2.209338
84	6	0	-21.056736	4.854047	-1.577671
85	6	0	-20.332191	3.628737	-1.006582
86	6	0	-18.820549	3.659523	-1.278349
87	6	0	-18.087661	2.436015	-0.705460
88	6	0	-16.573970	2.468949	-0.971043
89	6	0	-15.841436	1.250117	-0.387530
90	6	0	-14.325172	1.288835	-0.636882
91	6	0	-13.593407	0.080541	-0.030949
92	6	0	-12.072752	0.132653	-0.251631
93	6	0	-11.339676	-1.051639	0.401733
94	6	0	-14.326554	-13.201938	-3.026470
95	6	0	-14.121138	-11.775516	-3.551477
96	6	0	-13.254994	-10.922440	-2.612393
97	6	0	-13.046628	-9.490300	-3.130109
98	6	0	-12.184424	-8.636025	-2.186875
99	6	0	-11.982841	-7.200814	-2.698900
100	6	0	-11.131705	-6.344187	-1.747781
101	6	0	-10.943997	-4.903423	-2.248998
102	6	0	-10.113909	-4.043085	-1.282341
103	6	0	-9.941804	-2.593541	-1.771382
104	1	0	3.805151	-3.612752	-0.317792
105	1	0	1.450978	-4.018679	-0.336935
106	1	0	2.757390	3.074835	-0.190768
107	1	0	-0.802502	-4.224762	-0.317225
108	1	0	-3.190124	-4.252595	-0.265171
109	1	0	-3.373077	2.514487	-0.188847
110	1	0	7.257368	-0.985364	1.561721
111	1	0	7.044166	1.706199	-1.747447
112	1	0	-7.066193	0.366963	1.667964
113	1	0	-7.331309	-2.264211	-1.685656
114	1	0	12.088104	14.425441	-3.982749
115	1	0	10.578395	14.022506	-3.131817
116	1	0	12.146475	13.835464	-2.305150
117	1	0	12.787964	12.016053	-3.936772
118	1	0	11.222376	12.202912	-4.762083
119	1	0	10.030742	11.529944	-2.655334
120	1	0	11.597565	11.342898	-1.829596
121	1	0	12.247217	9.553612	-3.468322
122	1	0	10.679617	9.740025	-4.292856
123	1	0	9.491229	9.070959	-2.184499
124	1	0	11.058654	8.885125	-1.359921
125	1	0	11.706927	7.094500	-2.997770
126	1	0	10.137597	7.279223	-3.819651
127	1	0	8.953175	6.613957	-1.707902
128	1	0	10.522019	6.431002	-0.885673
129	1	0	11.168119	4.636356	-2.520114
130	1	0	9.595862	4.816914	-3.338603
131	1	0	8.419858	4.159219	-1.215637
132	1	0	9.987393	3.987182	-0.400898

133	1	0	10.603603	2.180093	-2.133463
134	1	0	9.020235	2.360497	-2.829555
135	1	0	22.869589	-2.749905	-1.588832
136	1	0	21.595098	-3.970384	-1.360928
137	1	0	21.694798	-3.058094	-2.889036
138	1	0	21.148115	-0.925209	-1.649478
139	1	0	21.048944	-1.836400	-0.124102
140	1	0	19.141331	-3.182638	-1.052554
141	1	0	19.238772	-2.267775	-2.577555
142	1	0	18.722948	-0.145672	-1.338636
143	1	0	18.631253	-1.058741	0.187562
144	1	0	16.724359	-2.408289	-0.736859
145	1	0	16.810393	-1.486103	-2.258208
146	1	0	16.297225	0.628453	-1.008646
147	1	0	16.226950	-0.288333	0.516384
148	1	0	14.315718	-1.644968	-0.392699
149	1	0	14.373806	-0.708226	-1.906687
150	1	0	13.867239	1.392110	-0.631595
151	1	0	13.836437	0.463064	0.888101
152	1	0	11.930143	-0.911907	-0.009630
153	1	0	11.924599	0.062066	-1.492731
154	1	0	11.467764	2.126258	-0.128841
155	1	0	11.487614	1.231671	1.331428
156	1	0	13.760653	-12.184133	5.426660
157	1	0	12.168566	-12.045632	4.644356
158	1	0	13.655837	-11.818442	3.688535
159	1	0	14.197994	-9.745545	5.027721
160	1	0	12.713064	-9.972614	5.981991
161	1	0	11.333247	-9.703407	3.900126
162	1	0	12.819168	-9.475742	2.945134
163	1	0	13.372265	-7.430061	4.292731
164	1	0	11.887664	-7.658785	5.249513
165	1	0	10.506409	-7.394793	3.169133
166	1	0	11.990844	-7.164083	2.212761
167	1	0	12.541213	-5.117765	3.558897
168	1	0	11.059096	-5.349987	4.518945
169	1	0	9.673016	-5.091202	2.440805
170	1	0	11.154817	-4.855499	1.481920
171	1	0	11.702261	-2.809673	2.828355
172	1	0	10.219282	-3.042526	3.788467
173	1	0	8.840930	-2.808467	1.698690
174	1	0	10.317230	-2.553460	0.751523
175	1	0	10.847549	-0.546670	2.237608
176	1	0	9.292185	-0.736143	3.019360
177	1	0	-11.245246	12.402402	5.975393
178	1	0	-9.732513	11.978808	5.139874
179	1	0	-11.259019	12.081183	4.225384
180	1	0	-12.166850	10.112453	5.523436
181	1	0	-10.642453	10.010453	6.436135
182	1	0	-9.397235	9.545148	4.304412
183	1	0	-10.923185	9.644747	3.391655
184	1	0	-11.833000	7.703258	4.698687
185	1	0	-10.309066	7.606020	5.615326
186	1	0	-9.058761	7.149063	3.485502
187	1	0	-10.584276	7.238668	2.571207
188	1	0	-11.483671	5.292692	3.876096

189	1	0	-9.963216	5.208143	4.799974
190	1	0	-8.699835	4.761660	2.674622
191	1	0	-10.223154	4.832064	1.755520
192	1	0	-11.105538	2.880466	3.060808
193	1	0	-9.587548	2.813074	3.991705
194	1	0	-8.314310	2.402607	1.861329
195	1	0	-9.832603	2.429019	0.947743
196	1	0	-10.672392	0.507054	2.390123
197	1	0	-9.101260	0.409780	3.158742
198	1	0	-22.139146	4.811564	-1.371639
199	1	0	-20.670151	5.787310	-1.135671
200	1	0	-20.928262	4.919076	-2.670875
201	1	0	-20.765055	2.713393	-1.449104
202	1	0	-20.507172	3.580537	0.083366
203	1	0	-18.393017	4.578359	-0.836986
204	1	0	-18.649716	3.707629	-2.369322
205	1	0	-18.513667	1.517545	-1.148764
206	1	0	-18.262793	2.387592	0.384784
207	1	0	-16.149811	3.390358	-0.531999
208	1	0	-16.396843	2.511390	-2.061158
209	1	0	-16.258960	0.328190	-0.831667
210	1	0	-16.027365	1.204700	0.701111
211	1	0	-13.911660	2.216988	-0.201998
212	1	0	-14.134943	1.320974	-1.725040
213	1	0	-13.994818	-0.849129	-0.474052
214	1	0	-13.797793	0.044047	1.054838
215	1	0	-11.688134	1.080954	0.160168
216	1	0	-11.857945	0.141678	-1.335026
217	1	0	-11.750707	-1.988989	-0.003624
218	1	0	-11.604977	-1.125993	1.469435
219	1	0	-14.950068	-13.796382	-3.714703
220	1	0	-13.363600	-13.726793	-2.912034
221	1	0	-14.827345	-13.196509	-2.044129
222	1	0	-15.106450	-11.292199	-3.680428
223	1	0	-13.645270	-11.821343	-4.547717
224	1	0	-12.270947	-11.409676	-2.485686
225	1	0	-13.733380	-10.882473	-1.616744
226	1	0	-14.031495	-9.005434	-3.259116
227	1	0	-12.566039	-9.530197	-4.124584
228	1	0	-11.197889	-9.117995	-2.060680
229	1	0	-12.663628	-8.601014	-1.191505
230	1	0	-12.970352	-6.722144	-2.830913
231	1	0	-11.497042	-7.233564	-3.691119
232	1	0	-10.140684	-6.816529	-1.621224
233	1	0	-11.614629	-6.320621	-0.753833
234	1	0	-11.936791	-4.436579	-2.385675
235	1	0	-10.448957	-4.922299	-3.237077
236	1	0	-9.116750	-4.498702	-1.149181
237	1	0	-10.602235	-4.044673	-0.291703
238	1	0	-10.917964	-2.150074	-2.024725
239	1	0	-9.395919	-2.606636	-2.731435

DFT calculation data for **PBI-Se[10] :**

Center	Atomic	Atomic	Coordinates (Angstroms)		
No.	No.	Type	X	Y	Z

1	6	0	-3.109191	2.206517	0.377847
2	6	0	-1.739158	2.352105	0.634949
3	6	0	-0.788413	1.538941	0.008023
4	6	0	-1.282026	0.559492	-0.910434
5	6	0	-2.664815	0.408623	-1.174594
6	6	0	-3.581590	1.247377	-0.513390
7	6	0	-0.399489	-0.304755	-1.585451
8	6	0	-0.824932	-1.281265	-2.488590
9	6	0	-2.200243	-1.424310	-2.749208
10	6	0	-3.098650	-0.590299	-2.096123
11	6	0	0.669420	1.620839	0.238253
12	6	0	1.525416	0.717561	-0.467413
13	6	0	0.993072	-0.226248	-1.365814
14	6	0	1.286572	2.521978	1.113010
15	6	0	2.676593	2.531486	1.291750
16	6	0	3.501968	1.646227	0.604302
17	6	0	2.930388	0.724254	-0.292380
18	6	0	3.733379	-0.203126	-1.020658
19	6	0	3.175792	-1.119378	-1.903234
20	6	0	1.779673	-1.134063	-2.078118
21	6	0	-4.551052	-0.754342	-2.370844
22	7	0	-5.435558	0.088083	-1.653624
23	6	0	-5.039731	1.101159	-0.745764
24	6	0	4.967809	1.665983	0.832047
25	7	0	5.734066	0.724582	0.100295
26	6	0	5.209226	-0.199908	-0.836155
27	8	0	-5.862103	1.801475	-0.180506
28	8	0	-4.971548	-1.585781	-3.157743
29	8	0	5.492757	2.441321	1.612933
30	8	0	5.939144	-0.962559	-1.446879
31	6	0	-6.856692	-0.101639	-1.862633
32	6	0	7.164247	0.703953	0.332465
33	6	0	-7.450203	-1.307674	-1.519774
34	6	0	-8.821691	-1.509737	-1.704835
35	6	0	-9.621673	-0.473083	-2.240706
36	6	0	-9.003714	0.752646	-2.599997
37	6	0	-7.628117	0.917033	-2.407938
38	6	0	7.766851	-0.441684	0.833600
39	6	0	9.144091	-0.482304	1.076760
40	6	0	9.929354	0.672319	0.848262
41	6	0	9.305178	1.835185	0.336041
42	6	0	7.932695	1.832093	0.072331
43	34	0	0.674370	-2.227028	-3.168059
44	6	0	-16.006018	11.304474	-0.554571
45	6	0	-15.298281	10.421128	-1.585899
46	6	0	-14.593031	9.209364	-0.965347
47	6	0	-13.887121	8.315197	-1.991271
48	6	0	-13.189889	7.099834	-1.369351
49	6	0	-12.492534	6.197771	-2.394530
50	6	0	-11.806799	4.977367	-1.769493
51	6	0	-11.119765	4.064925	-2.792610
52	6	0	-10.443059	2.843551	-2.160536
53	6	0	-9.755585	1.932401	-3.196521
54	6	0	-21.253009	-1.854263	3.015353
55	6	0	-20.438283	-1.708956	1.727040

56	6	0	-18.933480	-1.549576	1.975290
57	6	0	-18.109489	-1.407002	0.690547
58	6	0	-16.604580	-1.252524	0.939610
59	6	0	-15.779049	-1.122272	-0.345691
60	6	0	-14.273365	-0.975614	-0.095857
61	6	0	-13.445224	-0.866552	-1.381560
62	6	0	-11.939706	-0.723881	-1.129126
63	6	0	-11.114837	-0.682714	-2.434014
64	6	0	-11.288593	-9.424225	8.054913
65	6	0	-11.348460	-9.218794	6.538614
66	6	0	-10.843844	-7.841321	6.092273
67	6	0	-10.894142	-7.628768	4.574908
68	6	0	-10.389496	-6.250458	4.132118
69	6	0	-10.424574	-6.038566	2.613997
70	6	0	-9.916556	-4.658934	2.179082
71	6	0	-9.927207	-4.445215	0.660699
72	6	0	-9.412859	-3.063723	0.241512
73	6	0	-9.372119	-2.864427	-1.287568
74	6	0	11.661867	-12.827545	-1.313685
75	6	0	11.675090	-11.684417	-0.295058
76	6	0	11.202041	-10.346304	-0.876012
77	6	0	11.210201	-9.199119	0.140605
78	6	0	10.734975	-7.859803	-0.435169
79	6	0	10.735736	-6.719762	0.589762
80	6	0	10.255453	-5.378057	0.023521
81	6	0	10.242218	-4.249780	1.061506
82	6	0	9.751972	-2.907247	0.507797
83	6	0	9.707326	-1.800925	1.581609
84	6	0	21.755987	-1.901409	-3.398320
85	6	0	20.895158	-1.358842	-2.254042
86	6	0	19.392618	-1.386576	-2.558687
87	6	0	18.523604	-0.846007	-1.417355
88	6	0	17.021205	-0.874372	-1.721381
89	6	0	16.153341	-0.336544	-0.577595
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91	6	0	13.784303	0.166865	0.267801
92	6	0	12.281755	0.135882	-0.032970
93	6	0	11.423062	0.673229	1.130222
94	6	0	12.684083	12.898772	5.769877
95	6	0	12.737182	12.054777	4.493289
96	6	0	12.046529	10.693414	4.638384
97	6	0	12.092306	9.838344	3.366810
98	6	0	11.398634	8.479703	3.520667
99	6	0	11.436977	7.615520	2.254831
100	6	0	10.736777	6.262108	2.425978
101	6	0	10.762266	5.381483	1.171118
102	6	0	10.051895	4.038245	1.372476
103	6	0	10.050237	3.141278	0.117613
104	1	0	-3.837435	2.838543	0.874561
105	1	0	-1.422323	3.112573	1.340098
106	1	0	-2.601846	-2.159352	-3.437953
107	1	0	0.687202	3.230614	1.673802
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109	1	0	3.847510	-1.792785	-2.424089
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113	1	0	7.458203	2.728630	-0.311037
114	1	0	-16.501295	12.157460	-1.029612
115	1	0	-16.768798	10.739829	-0.006447
116	1	0	-15.297357	11.699509	0.182314
117	1	0	-14.564771	11.021003	-2.141831
118	1	0	-16.026594	10.072673	-2.331024
119	1	0	-15.326625	8.611354	-0.405542
120	1	0	-13.861936	9.557707	-0.221365
121	1	0	-13.150335	8.911713	-2.548205
122	1	0	-14.618452	7.971551	-2.737005
123	1	0	-13.926524	6.507720	-0.807547
124	1	0	-12.454460	7.443249	-0.627644
125	1	0	-11.750229	6.786270	-2.952533
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130	1	0	-11.858741	3.729862	-3.534923
131	1	0	-11.185081	2.267447	-1.594919
132	1	0	-9.694397	3.172308	-1.427658
133	1	0	-9.038424	2.539874	-3.760994
134	1	0	-10.498476	1.593672	-3.927854
135	1	0	-22.321253	-1.966866	2.803919
136	1	0	-20.933085	-2.731250	3.589523
137	1	0	-21.132212	-0.977189	3.661353
138	1	0	-20.804304	-0.844072	1.156991
139	1	0	-20.607904	-2.584236	1.085152
140	1	0	-18.567429	-2.413881	2.548060
141	1	0	-18.762847	-0.672779	2.616595
142	1	0	-18.474351	-0.541408	0.119081
143	1	0	-18.283017	-2.283148	0.049294
144	1	0	-16.242059	-2.114746	1.517423
145	1	0	-16.429462	-0.372518	1.574958
146	1	0	-16.138273	-0.258063	-0.922717
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150	1	0	-13.798602	-0.008670	-1.971634
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154	1	0	-11.520567	0.102053	-3.077245
155	1	0	-11.283871	-1.621931	-2.974274
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159	1	0	-12.381295	-9.355886	6.190258
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162	1	0	-11.436695	-7.059856	6.589239
163	1	0	-11.925890	-7.769710	4.222105
164	1	0	-10.299629	-8.409675	4.079294
165	1	0	-9.360918	-6.107535	4.493185
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167	1	0	-11.452099	-6.181070	2.249875

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169	1	0	-8.893929	-4.514407	2.555848
170	1	0	-10.524555	-3.879419	2.659979
171	1	0	-10.948149	-4.588345	0.278432
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176	1	0	-8.738806	-3.648433	-1.722932
177	1	0	12.004937	-13.766402	-0.867132
178	1	0	10.653107	-12.995744	-1.707680
179	1	0	12.314443	-12.606580	-2.165990
180	1	0	12.689815	-11.564282	0.108523
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182	1	0	10.187160	-10.466358	-1.281877
183	1	0	11.836655	-10.078923	-1.733234
184	1	0	12.225460	-9.079896	0.545582
185	1	0	10.576959	-9.469657	0.997779
186	1	0	9.721779	-7.979619	-0.844799
187	1	0	11.371552	-7.584001	-1.287998
188	1	0	11.749359	-6.599148	0.998383
189	1	0	10.101515	-6.999605	1.443204
190	1	0	9.245557	-5.499701	-0.393134
191	1	0	10.895125	-5.089145	-0.822431
192	1	0	11.252629	-4.125603	1.477149
193	1	0	9.606068	-4.544940	1.908533
194	1	0	8.751821	-3.030165	0.072660
195	1	0	10.397877	-2.586984	-0.320209
196	1	0	10.710777	-1.670497	1.993889
197	1	0	9.082800	-2.153697	2.413532
198	1	0	22.821646	-1.866698	-3.149924
199	1	0	21.501303	-2.942689	-3.626518
200	1	0	21.608841	-1.319223	-4.315151
201	1	0	21.198291	-0.328235	-2.024012
202	1	0	21.089690	-1.938976	-1.341609
203	1	0	19.088963	-2.417742	-2.790391
204	1	0	19.197270	-0.805649	-3.471650
205	1	0	18.827925	0.185030	-1.186428
206	1	0	18.720399	-1.426940	-0.504819
207	1	0	16.717082	-1.904941	-1.954287
208	1	0	16.823640	-0.291435	-2.632387
209	1	0	16.456749	0.694444	-0.345469
210	1	0	16.352185	-0.918702	0.333664
211	1	0	14.347301	-1.396469	-1.115020
212	1	0	14.450305	0.219228	-1.788225
213	1	0	14.086889	1.197484	0.503041
214	1	0	13.985519	-0.417707	1.177156
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223	1	0	12.272635	12.609688	3.666754

224	1	0	10.998961	10.848988	4.934271
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227	1	0	11.627747	10.392566	2.538641
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231	1	0	10.971479	8.164694	1.423906
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233	1	0	11.202794	5.716735	3.259116
234	1	0	11.804693	5.205119	0.868843
235	1	0	10.294545	5.921334	0.335301
236	1	0	9.012481	4.211577	1.680218
237	1	0	10.520091	3.497263	2.205656
238	1	0	11.080901	2.961642	-0.205512
239	1	0	9.567537	3.687617	-0.701662

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